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ANTI-IL-13 ANTIBODIES AND COMPLEXES

Abstract:

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(A2) Translate this text Anti-IL-13 antibodies, crystals of anti-IL-13 antibodies, IL-13 polypeptide/anti-IL-13 antibody complexes, crystals of IL-13 polypeptide/anti-IL-13 antibody complexes, IL-13Ralpha1 polypeptide/IL-13 polypeptide/anti-IL-13 antibody complexes, crystals of IL-13Ralpha1 polypeptide/IL-13 polypeptide/anti-IL-13 antibody complexes, and related methods and software systems are disclosed.

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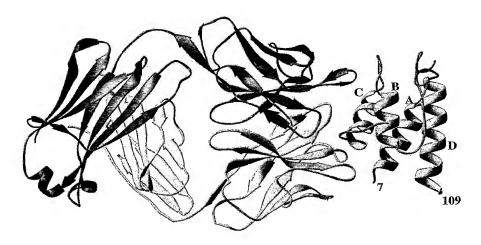
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(54) Title: ANTI-IL-13 ANTIBODIES AND COMPLEXES



(57) Abstract: Anti-IL-13 antibodies, crystals of anti-IL-13 antibodies, IL-13 polypeptide/anti-IL-13 antibody complexes, crystals of IL-13 polypeptide/anti-IL-13 antibody complexes, IL-13Rα1 polypeptide/IL-13 polypeptide/IL-13 antibody complexes, crystals of IL-13Rα1 polypeptide/IL-13 polypeptide/IL-13 antibody complexes, and related methods and software systems are disclosed.

ANTI-IL-13 ANTIBODIES AND COMPLEXES

RELATED APPLICATIONS

This application claims the benefit of U.S. Provisional Application Number 60/578,736, filed June 9, 2004, U.S. Provisional Patent Application No. 60/578,473, filed June 9, 2004, and U.S. Provisional Patent Application No. 60/581,375 filed June 22, 2004. The contents of each of these applications are incorporated herein by reference in their entirety.

TECHNICAL FIELD

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The invention relates to anti-IL-13 antibodies, crystals of anti-IL-13 antibodies, IL-13 polypeptide/anti-IL-13 antibody complexes, crystals of IL-13 polypeptide/anti-IL-13 antibody complexes, IL-13Rα1 polypeptide/IL-13 polypeptide/anti-IL-13 antibody complexes, crystals of IL-13Rα1 polypeptide/IL-13 polypeptide/anti-IL-13 antibody complexes, and related methods and software systems.

BACKGROUND

Interleukin-13 (IL-13) is a pleiotropic cytokine involved in immune response conditions, such as atopy, asthma, allergy, and inflammatory response. The role of IL-13 in immune response is facilitated by its effect on cell-signaling pathways. For example, IL-13 can promote B cell proliferation, induce B cells to produce IgE, and down regulate the production of proinflammatory cytokines. IL-13 can also increase expression of VCAM-1 on endothelial cells, and enhance expression of class II MHC antigens and various adhesion molecules on monocytes.

IL-13 function is mediated through an interaction with its receptor on hematopoietic and other cell types. The human IL-13 receptor (IL-13R) is a heterodimer that includes the interleukin-4 receptor α chain, IL-4R α , and the IL-13 binding chain, IL-13R α 1. The association of IL-13 with its receptor induces the activation of STAT6 (signal transducer and activation of transcription 6) and JAK1 (Janus-family kinase) through a binding interaction with the IL-4R α chain. IL-13R α 2, which may be found on the cell surface or in soluble form in the circulation,

binds to IL-13 with high affinity but does not mediate cellular responses to IL-13. It is thought to function as a decoy receptor.

SUMMARY

In one aspect, the invention features a crystalline antibody. The crystalline antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

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In another aspect, the invention features a crystalline composition that includes an antibody. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

In a further aspect, the invention features a crystalline complex that includes an IL-13 polypeptide and an antibody. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

In another aspect, the invention features a crystalline complex that includes an IL-13R α 1 polypeptide and an IL-13 polypeptide.

In yet another aspect, the invention features a method that includes using a three-dimensional model of an antibody to design an agent that interacts with an IL-13 polypeptide. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

In another aspect, the invention features a method that includes using a three-dimensional model of an IL-13 polypeptide to design an agent that interacts with the IL-13 polypeptide.

In another aspect, the invention features a method that includes using a three-dimensional model of an IL-13 polypeptide bound to an IL-13R α 1 polypeptide to design an agent that interacts with the IL-13 polypeptide.

In another aspect, the invention features a method that includes selecting an agent by performing rational drug design with a three-dimensional structure of a crystalline complex that includes an IL-13 polypeptide; contacting the agent with an IL-13 polypeptide; and detecting the ability of the agent to bind the IL-13 polypeptide.

In a further aspect, the invention features a method that includes contacting an IL-13 polypeptide with an antibody to form a composition; and crystallizing the composition to form a crystalline complex in which the antibody is bound to the IL-13 polypeptide. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-

13 antibody, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

In another aspect, the invention features a method that includes contacting an IL-13 polypeptide with an antibody and an IL-13Rα1 polypeptide to form a composition, and crystallizing the composition to form a crystalline complex in which the antibody and the IL-13Rα1 polypeptide are each bound to the IL-13 polypeptide. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

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In another aspect, the invention features a software system that includes instructions for causing a computer system to accept information relating to a structure of an IL-13 polypeptide bound to an antibody, the antibody including an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody. The instructions also cause the computer system to accept information relating to a candidate agent and to determine binding characteristics of the candidate agent to the IL-13 polypeptide. The determination of binding characteristics is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent.

In another aspect, the invention features a computer program residing on a computer readable medium. A plurality of instructions is stored on the computer readable medium. When the instructions are executed by one or more processors, the one or more processors will accept information relating to a structure of an IL-13 polypeptide bound to an antibody, the antibody being an anti-IL-13 polypeptide or a Fab fragment of an anti-IL-13 antibody; accept information relating to a candidate agent; and determine binding characteristics of the candidate agent to the IL-13 polypeptide. Determination of the binding characteristics is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent.

In another aspect, the invention features a method that includes accepting information relating to the structure of an IL-13 polypeptide bound to an antibody and modeling the binding characteristics of the IL-13 polypeptide with a candidate agent. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody. The method of accepting information and modeling the binding characteristics is implemented by a software system.

In another aspect, the invention features a computer program residing on a computer readable medium containing a plurality of instructions. When the instructions are executed by one or more processors, the one or more processors will accept information relating to the structure of an IL-13 polypeptide bound to an antibody, the antibody being an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody; and model the binding characteristics of the IL-13 polypeptide with a candidate agent.

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In another aspect, the invention features a software system, that includes instructions for causing a computer system to accept information relating to the structure of an IL-13 polypeptide bound to an antibody, and model the binding characteristics of the IL-13 polypeptide with a candidate agent. The antibody is an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

In another aspect, the invention features a crystalline antibody. The antibody is capable of binding to a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

In a further aspect, the invention features a crystalline composition that includes an antibody capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

In another aspect, the invention features a crystalline complex that includes an IL-13 polypeptide and an antibody. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

In yet another aspect, the invention features a crystalline complex that includes an IL-13 polypeptide, an IL-13Ra1 polypeptide, and an antibody. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds in vivo.

In another aspect, the invention features a method that includes using a three-dimensional model of an antibody to design an agent that interacts with an IL-13 polypeptide. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

In another aspect, the invention features a method that includes contacting an IL-13 polypeptide with an antibody to form a composition; and crystallizing the composition to form a crystalline complex in which the antibody is bound to the IL-13 polypeptide. The antibody is capable of binding a site of an IL-13 polypeptide to

which an IL-4R polypeptide binds *in vivo*, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

In yet another aspect, the invention features a method that includes contacting an IL-13 polypeptide with an antibody and an IL-13Rα1 polypeptide to form a composition, and crystallizing the composition to form a crystalline complex in which the antibody and the IL-13Rα1 polypeptide are each bound to the IL-13 polypeptide. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

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In another aspect, the invention features a software system that includes instructions for causing a computer system to accept information relating to a structure of an IL-13 polypeptide bound to an antibody, accept information relating to a candidate agent, and determine binding characteristics of the candidate agent to the IL-13 polypeptide. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds in vivo. The determination of binding characteristics of the candidate agent is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent.

In another aspect, the invention features a computer program residing on a computer readable medium containing a plurality of instructions. When the instructions are executed by one or more processors, the one or more processors will accept information relating to a structure of an IL-13 polypeptide bound to an antibody, accept information relating to a candidate agent; and determine the binding characteristics of the candidate agent to the IL-13 polypeptide. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds in vivo. Determination of the binding characteristics of the candidate agent is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent

In another aspect, the invention features a method that includes accepting information relating to the structure of an IL-13 polypeptide bound to an antibody and modeling the binding characteristics of the IL-13 polypeptide with a candidate agent. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*. The method of accepting information and modeling the binding characteristics is implemented by a software system.

In another aspect, the invention features a computer program residing on a computer readable medium containing a plurality of instructions. When the instructions are executed by one or more processors, the one or more processors will accept information relating to the structure of an IL-13 polypeptide bound to an antibody and model the binding characteristics of the IL-13 polypeptide with a candidate agent. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

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In another aspect, the invention features a software system that includes instructions for causing a computer system to accept information relating to the structure of an IL-13 polypeptide bound to an antibody and model the binding characteristics of the IL-13 polypeptide with a candidate agent. The antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds in vivo.

In another aspect, the invention features a method of modulating IL-13 activity in a subject. The method includes using rational drug design to select an agent that is capable of modulating IL-13 activity, and administering a therapeutically effective amount of the agent to the subject.

In a further aspect, the invention features a method of treating a subject having a condition associated with IL-13 activity. The method includes using rational drug design to select an agent that is capable of effecting IL-13 activity, and administering a therapeutically effective amount of the agent to the subject.

In another aspect, the invention features a method of prophylactically treating a subject susceptible to a condition associated with IL-13 activity. The method includes determining that the subject is susceptible to the condition associated with IL-13 activity, using rational drug design to select an agent that is capable of effecting IL-13 activity, and administering a therapeutically effective amount of the agent to the subject.

Structural information of a polypeptide or a corresponding ligand can lead to a greater understanding of how the polypeptide functions *in vivo*. For example, knowledge of the structure of a protein or a corresponding ligand can reveal properties that facilitate the interaction of the protein with its ligands, including other proteins, antibodies, effector molecules (*e.g.*, hormones), and nucleic acids. Structure based modeling can be used to identify ligands capable of interacting with an IL-13

polypeptide, thus eliminating the need for screening assays, which can be expensive and time-consuming. Structural information can also be used to direct the modification of a ligand known to interact with IL-13 to generate an alternative ligand with more desirable properties, such as tighter binding or greater specificity.

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The study of the interaction between an anti-IL-13 antibody and an IL-13 polypeptide and between an IL-13 polypeptide and its receptor can facilitate the design or selection of ligands (e.g., drugs) for modulating the activity of IL-13 in vivo. Such studies can therefore be useful for designing therapeutic agents. Activity assays indicated that mAb13.2 blocked IL-13 function in vitro and in vivo (see Examples 1 and 2 below), including the use of an antibody to identify IL-13-binding agents capable of disturbing the normal function of the protein. Accordingly, it is believed that the crystal structures of the mAb13.2Fab fragment, the human IL-13/mAb13.2 Fab fragment complex, and the human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex (see Tables 10-12 below) can be useful for designing or identifying agents that can interact with IL-13 and the IL-13 receptor polypeptide, IL-13Rα1. Such agents may be useful in modulating the activity of IL-13 in immune response conditions, such as, for example, asthma (e.g., nonallergic asthma, or allergic asthma, which is sometimes referred to as chronic allergic airway disease), chronic obstructive pulmonary disorder (COPD), airway inflammation, eosinophilia, fibrosis and excess mucus production (e.g., cystic fibrosis, pulmonary fibrosis, and allergic rhinitis), inflammatory and/or autoimmune conditions of the skin (e.g., atopic dermatitis), inflammatory and/or autoimmune conditions of the gastrointestinal organs (e.g., inflammatory bowel disease (IBD) and/or Crohn's disease), liver (e.g., cirrhosis), inflammatory and/or autoimmune conditions of the blood vessels or connective tissue (e.g., scleroderma), and tumors or cancers (e.g., soft tissue or solid tumors), such as Hodgkin's lymphoma, glioblastoma, and lymphoma.

Other features and advantages of the invention will be apparent from the accompanying drawings and description, and from the claims. The contents of all references, pending patent applications and published patents, cited throughout this application are hereby expressly incorporated by reference. In case of conflict, the present application, including definitions, will control.

DESCRIPTION OF DRAWINGS

FIG. 1A is the amino acid sequence of the light chain of the mAb13.2 Fab (fragment antigen binding) fragment (SEQ ID NO:1).

FIG. 1B is the amino acid sequence of the heavy chain of mAb13.2 Fab fragment (SEQ ID NO:2).

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FIG. 2A is the amino acid sequence of full-length human IL-13 (Swiss-Prot Accession No. P35225) (SEQ ID NO:3). The signal peptide cleavage site is indicated by a slash. Alpha helices A, B, C, and D are underlined. Helix A is defined by amino acids 25-42; helix B is defined by amino acids 62-71; helix C is defined by amino acids 78-89; and helix D is defined by amino acids 112-127.

FIG. 2B is the amino acid sequence of human IL-13 (SEQ ID NO:4) following cleavage of the signal peptide. Alpha helices A, B, C, and D are underlined. Helix A is defined by amino acids 6-23; helix B is defined by amino acids 43-52; helix C is defined by amino acids 59-70; helix D is defined by amino acids 93-108.

FIG. 3 is a ribbon diagram illustrating the crystal structure of mAb13.2 Fab fragment (left) with the processed form of human IL-13 (right) (see FIG. 2B). The light chain of mAb13.2 Fab fragment is shown in dark shading, and the heavy chain in light shading. Helices A, B, C, and D of the IL-13 structure are indicated.

FIG. 4 is a graph illustrating the kinetic parameters of three different anti-IL-13 antibodies (mAb13.2, mAb13.4, and mAb13.9) binding to human IL-13 as determined by Biacore analyses. Kinetic constants for mAb13.2 are also shown.

FIG. 5 is a graph illustrating the binding of biotinylated mAb13.2 to recombinant and native human IL-13. ELISA plates were coated with anti-FLAG M2 antibody. The binding of FLAG-human IL-13 was detected with biotinylated mAb13.2 and streptavidin-peroxidase. This binding could be competed with native human IL-13 isolated from mitogen activated, Th2-skewed, cord blood mononuclear cells (triangles); and recombinant human IL-13 (diamonds). There was no detectable binding of recombinant murine IL-13 (circles) to mAb13.2.

FIG. 6 is a graph illustrating the effect of mAb13.2 and the known inhibitor rhuIL-13R α 2 on the bioactivity of human IL-13. "cpm" is the measure of ³H-thymidine taken up into TF1 cells grown in the presence of IL-13 and varying concentrations of mAb13.2 or rhuIL-13R α 2 (x-axis).

FIG. 7A is a graph illustrating the effect of recombinant human IL-13 and IL-4 on CD23 expression on CD11b+ monocytes. The monocytes were normal peripheral blood mononuclear cells (PBMCs) harvested from a healthy donor. The cells were treated overnight with 1 ng/mL recombinant human IL-13 or IL-4, then assayed for CD23 expression by flow cytometry.

FIG. 7B is a graph illustrating the effect of mAb13.2 on IL-13-induced CD23 expression on CD11b+ monocytes.

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FIG. 7C is a graph illustrating the effect of mAb13.2 on IL-4 - induced CD23 expression on CD11b+ monocytes.

FIG. 8 is a graph illustrating the effect of mAb13.2 on IL-13-dependent IgE production by human B cells. PBMC from a healthy donor were stimulated with PHA and IL-13. After 3 weeks, each well was assayed for IgE concentrations by ELISA. PHA + IL-13 increased the frequency of IgE-producing B cell clones. This effect was inhibited by mAb13.2, but not by an IL-13 specific nonneutralizing antibody (mAb13.8) or by control mouse IgG (msIgG).

FIG. 9A is a Western blot detecting phosphorylated STAT6 protein from HT-29 human epithelial cells treated with the indicated concentration of IL-13 for 30 min at 37° C.

FIG. 9B is a histogram from flow cytometry experiments that measured the level of cellular phosphorylated STAT6 protein following treatment with IL-13. The shift in phospho-STAT6 staining intensity upon treatment with IL-13 is indicated by the lightly shaded trace.

FIG. 9C is a panel of histograms from flow cytometry experiments that measured the level of cellular phosphorylated STAT6 protein following treatment with a sub-optimal concentration of human IL-13 and the indicated antibody. Cells treated with IL-13 and antibody are indicated by the bold trace. Shaded histograms indicate untreated cells. In addition to mAb13.2, an IL-13 specific nonneutralizing antibody (mAb13.8) and a control mouse IgG1 were also tested.

FIG. 10 is a graph demonstrating the percentage of eosinophils detected in BAL from Cynomolgus monkeys sensitized to *Ascaris suum* following lung segmental challenge with *Ascaris* antigen. Twenty-four hours before challenge, animals had been administered mAb13.2 i.v. (diamonds) or left untreated (circles). Triangles represent mAb13-2-treated and re-challenged with Ascaris at three months

post-Ab administration. Eosinophils were detected by flow cytometry using depolarized side scatter analysis.

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FIG. 11A is a graph showing that unlabeled mAb13.2 (diamonds) or mAb13.2 Fab fragments (circles) could compete for binding with biotinylated mAb13.2 in an ELISA assay. An "irrelevant antibody" (monoclonal antibody mAb13.8, which binds IL-13 but does not neutralize its activity) (asterisks) could not compete for binding. Competitor concentration is expressed as picomole (pM) antibody or Fab.

FIG. 11B is a graph showing that unlabeled mAb13.2 (diamonds) or mAb13.2 Fab fragment (circles) could compete for binding with biotinylated mAb13.2 in an ELISA assay. An "irrelevant antibody" (monoclonal antibody mAb13.8) (asterisks) could not compete for binding. Competitor concentration is expressed as picomole (pM) binding sites, assuming two binding sites per intact IgG and one binding site per Fab fragment.

FIG. 12A is a graph showing that mAb13.2 (diamonds) and mAb13.2 Fab fragment (circles) inhibited IL-13-dependent TF1 cell division. "Competitor concentration" is mAb13.2 and mAb13.2 Fab fragment concentration, and concentration is represented as pM competitor binding sites, assuming two binding sites per intact IgG and one binding site per Fab fragment.

FIG. 12B is a graph showing that mAb13.2 (diamonds) and mAb13.2 Fab fragment (circles) inhibited IL-13 CD23 expression on human PBMCs. Competitor concentration is mAb13.2 and mAb13.2 Fab fragment concentration, and the concentration is represented as pM competitor binding sites, assuming two binding sites per intact IgG and one binding site per Fab fragment.

FIG. 13 is the DNA sequence of the expression vector pAL-981 (SEQ ID NO:5), including a human IL-13 cDNA insert (hIL13coli). The cDNA sequence encoding IL-13 is underlined. Restriction sites Nde1 (nucleotide position 2722) and Xba1 (nucleotide position 3070) flank the cDNA sequence.

FIG. 14 is the amino acid sequence of human IL-13Rα1 (Swiss-Prot Accession No. P78552) (SEQ ID NO:12).

FIG. 15 is a ribbon diagram illustrating the structure of the mAb13.2 Fab/IL-13/IL-13Rα1 trimeric complex.

FIG. 16 is a ribbon diagram illustrating the interaction between IL-13 and Ig domain 1 of IL-13R α 1.

FIG. 17 is a ribbon diagram illustrating the interaction between IL-13 and Ig domain 3 of IL-13R α 1.

DETAILED DESCRIPTION

The structure of the antigen binding fragment (Fab) of a murine monoclonal anti-IL-13 antibody, mAb13.2, was discovered by X-ray crystallography (see Table 10 below). The crystal structures of human IL-13 complexed with the mAb13.2 Fab fragment, and of human IL-13 complexed with both the mAb13.2 Fab fragment and an IL-13Rα1 polypeptide fragment were also discovered by X-ray crystallography (See Tables 11 and 12 below, respectively).

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FIGs. 1A and 1B provide amino acid sequence information for the light and heavy chain polypeptides of the mAb13.2 Fab fragment. FIGs. 2A and 2B provide amino acid sequence information for human IL-13. FIG. 3 provides structural information for a crystal of a human IL-13/mAb13.2 Fab fragment complex. The mAb13.2 Fab fragment binds to the IL-4R (IL-4Rα) binding domain of human IL-13, which includes the amino acids Ser7, Thr8, Ala9, Glu12, Leu48, Glu49, Ile52, Asn53, Arg65, Met66, Ser68, Gly69, Phe70, Cys71, Pro72, His73, Lys74, and Arg86 as defined by SEQ ID NO:4.

FIG. 14 provides amino acid sequence information for the human IL-13 receptor polypeptide, human IL-13Rα1. FIGs. 15, 16, and 17 provide structural information for a crystal of a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. In addition to the interaction described above between human IL-13 and the mAb13.2 Fab fragment, human IL-13 forms two contacts with the human IL-13Rα1 polypeptide, one with Ig domain 1 of the human IL-13Rα1 polypeptide, and a second with the Ig domain 3 of the human IL-13Rα1 polypeptide. The interaction with Ig domain 1 involves residues Thr88, Lys89, Ile90, and Glu91 of human IL-13 as defined by SEQ ID NO:4, and residues Lys76, Lys77, Ile78, and Ala79 of the human IL-13Rα1 polypeptide, as defined by SEQ ID NO:12 (see FIG. 16). The interaction with Ig domain 3 involves residues Arg11, Glu12, Leu13, Ile14, Glu15, Lys104, Lys105, Leu106, Phe107, and Arg108 of human IL-13 as defined by SEQ ID NO:4, and residues Ile254, Ser255, Arg256, Lys318, Cys320, and Tyr321 of the human IL-13Rα1 polypeptide as defined by SEQ ID NO:12 (see FIG. 17).

In general, a crystal of the mAb13.2 Fab fragment can be prepared as desired. Typically, the process includes first isolating the mAb13.2 Fab fragment, and then

forming a crystal that contains that mAb13.2 Fab fragment. In some embodiments, a crystal containing the mAb13.2 Fab fragment can be prepared as follows. The intact antibody is cleaved with an appropriate proteolytic enzyme (e.g., papain), and the mAb13.2 Fab fragment is isolated from the Fc (Fragment crystallizable) fragment. The isolated mAb13.2 Fab fragment is disposed in an appropriate solution, and the solution is crystallized. The solution can contain, for example, one or more polymers (e.g., polyethylene glycol (PEG)), one or more salts (e.g., potassium sulfate) and optionally one or more organic solvents. The crystals can be grown by various methods, such as, for example, sitting or hanging drop vapor diffusion. In general, crystallization can be performed at a temperature of from about 4°C to 60°C (e.g., from about 4°C to about 45°C, such as at about 4°C, about 15°C, about 18°C, about 20°C, about 25°C, about 30°C, about 32°C, about 35°C, about 37°C). Structural data describing a crystal of the mAb13.2 Fab fragment can be obtained, for example, by Xray diffraction. X-ray diffraction data can be collected using a variety of means in order to obtain structural coordinates. Suitable X-ray sources include rotating anodes and synchrotron sources (e.g., Advanced Light Source (ALS), Berkeley, California; or Advanced Photon Source (APS), Argonne, Illinois). In certain embodiments, X-rays for generating diffraction data can have a wavelength of from about 0.5 Å to about 1.6 Å (e.g., about 0.7 Å, about 0.9 Å, about 1.0 Å, about 1.1 Å, about 1.3 Å, about 1.4 Å, about 1.5 Å, about 1.6 Å). Suitable X-ray detectors include area detectors and/or charge-couple devices (CCDs) can be used as the detector(s).

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In general, a crystal of the mAb13.2 Fab fragment can diffract X-rays to a resolution of about 3.5 Å or less (e.g., about 3.2 Å or less, about 3.0 Å or less, about 2.8 Å or less, about 2.5 Å or less, about 2.4 Å or less, about 2.3 Å or less, about 2.2 Å or less, about 2.1 Å or less, about 2.0 Å or less, about 1.9 Å or less, about 1.8 Å or less, about 1.7 Å or less, about 1.6 Å or less, about 1.5 Å or less, about 1.4 Å or less). In some embodiments, a crystal of the mAb13.2 Fab fragment can diffract X-rays to a resolution of from about 1.6 Å to about 2.5 Å (e.g., from about 1.8 Å to about 2.2 Å).

In certain embodiments, a crystal of the mAb13.2 Fab fragment can be orthorhombic with space group P2₁2₁2₁, and unit cell dimensions a= 54.4, b= 98.0, c=108.5, and $\alpha=\beta=\gamma=90$ °C.

In general, a complex including human IL-13 and the mAb13.2 Fab fragment can be prepared and crystallized as desired. In some embodiments, the process is as

follows. Human IL-13 is expressed from a DNA plasmid. The expression can be driven by a promoter, such as an inducible promoter. Human IL-13 can be expressed as a fusion protein with a suitable tag (e.g., to facilitate isolation of human IL-13 from cells), such as a glutathione-S-transferase (GST), myc, HA, hexahistidine, or FLAG tag. A fusion protein can be cleaved at a protease site engineered into the fusion protein, such as at or near the site of fusion between the polypeptide and the tag. Human IL-13 can be mixed with the mAb13.2 Fab fragment prior to purification (e.g., prior to cleavage of a polypeptide tag), or human IL-13 can be mixed with the mAb13.2 Fab fragment after purification. In some embodiments, the mAb13.2 Fab fragment can be mixed with human IL-13 prior to purification and again following purification. In some embodiments, human IL-13 polypeptide and the mAb13.2 Fab fragment are combined in a solution for collecting spectral data for the complex, NMR data for the complex, or for growing a crystal of the complex. The solution can contain, for example, one or more salts (e.g., a potassium salt), one or more polymers (e.g., polyethylene glycol (PEG)), and/or one or more organic solvents. Crystals can be grown by various methods, such as, for example, sitting or hanging drop vapor diffusion. In general, crystallization can be performed at about 16°C to 24°C (e.g., about 17°C to 23°C, or 18°C to 21°C).

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Structural information for a crystal of a human IL-13/mAb13.2 Fab fragment complex can be obtained by X-ray diffraction. In general, a crystal of a human IL-13/mAb13.2 Fab fragment complex can diffract X-rays to a resolution of about 3.5 Å or less (e.g., about 3.2 Å or less, about 3.0 Å or less, about 2.8 Å or less, about 2.5 Å or less, about 2.4 Å or less, about 2.3 Å or less, about 2.2 Å or less, about 2.1 Å or less, about 2.0 Å or less, about 1.9 Å or less, about 1.8 Å or less, about 1.7 Å or less, about 1.6 Å or less, about 1.5 Å or less, about 1.4 Å or less). In some embodiments, a crystal of a human IL-13/mAb13.2 Fab fragment complex can diffract X-rays to a resolution of from about 1.6 Å to about 2.5 Å (e.g., from about 1.8 Å to about 2.2 Å).

In certain embodiments, a crystal of a human IL-13/mAb13.2 Fab fragment complex can be cubic with space group P2₁3, and unit cell dimensions a= b= c= 125.3, and $\alpha=\beta=\gamma=90$ °C. The structure of the complex can be solved to a resolution of 1.8 Å.

In general, a complex including human IL-13, the mAb13.2 Fab fragment, and a human IL-13R α 1 polypeptide can be prepared and crystallized as desired. In some

embodiments, the process is as follows. A human IL-13Rα1 polypeptide is expressed from a DNA plasmid in the yeast strain *Pichia pastoris*, such that the expressed polypeptide is glycosylated. Expression from the DNA plasmid can be driven by a promoter, such as an inducible promoter. The human IL-13Rα1 polypeptide can be expressed as a fusion protein with a suitable tag (*e.g.*, to facilitate isolation of the human IL-13Rα1 polypeptide from cells), such as a glutathione-S-transferase (GST), myc, HA, hexahistidine, or FLAG tag. A fusion protein can be cleaved at a protease site engineered into the fusion protein, such as at or near the site of fusion between the polypeptide and the tag. The human IL-13Rα1 polypeptide can be mixed with human IL-13 to form a complex, and then the polypeptides of the complex can be deglycosylated by treatment with an enzyme such as endoglycosidase H. The mAb13.2 Fab fragment can be added to the deglycosylated complex to form a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab complex.

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In some embodiments, the human IL-13Rα1, human IL-13, and mAb13.2 Fab fragment are combined in a solution for collecting spectral data for the complex, NMR data for the complex, or for growing a crystal of the complex. The solution can contain, for example, one or more salts (*e.g.*, a potassium salt), one or more polymers (*e.g.*, polyethylene glycol (PEG)), and/or one or more organic solvents. Crystals can be grown by various methods, such as, for example, sitting or hanging drop vapor diffusion. In general, crystallization can be performed at about 16°C to 24°C (*e.g.*, about 17°C to 23°C, or 18°C to 21°C).

Structural information for a crystal of a human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex can be obtained by X-ray diffraction. In general, a crystal of a human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex can diffract X-rays to a resolution of about 3.5 Å or less (e.g., about 3.2 Å or less, about 3.0 Å or less, about 2.8 Å or less, about 2.5 Å or less, about 2.4 Å or less, about 2.3 Å or less, about 2.2 Å or less, about 2.1 Å or less, about 2.0 Å or less, about 1.9 Å or less, about 1.8 Å or less, about 1.7 Å or less, about 1.6 Å or less, about 1.5 Å or less, about 1.4 Å or less). In some embodiments, a crystal of a human IL-13/mAb13.2 Fab fragment complex can diffract X-rays to a resolution of from about 1.6 Å to about 2.5 Å (e.g., from about 1.8 Å to about 2.2 Å).

In certain embodiments, a crystal of a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex can be cubic with space group I4, and unit cell

dimensions a= b=164.9 Å, c= 74.8 Å, and $\alpha=\beta=\gamma=90^{\circ}\text{C}$. The structure of the complex can be solved to a resolution of 2.2 Å.

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X-ray diffraction data of a crystal of the mAb13.2 Fab fragment, human IL-13/mAb13.2 Fab fragment complex, or human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex can be used to obtain the structural coordinates of the atoms in the antibody or the complex. The structural coordinates are Cartesian coordinates that describe the location of atoms in three-dimensional space in relation to other atoms in the complex. As an example, the structural coordinates listed in Table 10 are the structural coordinates of a crystalline mAb13.2 Fab fragment. These structural coordinates describe the location of atoms of the mAb13.2 Fab fragment in relation to each other. As another example, the structural coordinates listed in Table 11 are the structural coordinates of a crystalline human IL-13/mAb13.2 Fab fragment complex. These structural coordinates describe the location of atoms of the human IL-13 in relation to each other, the location of atoms in the human IL-13 in relation to the atoms in the mAb13.2 Fab fragment, and the location of atoms in the mAb13.2 Fab fragment in relation to each other. As yet another example, the structural coordinates listed in Table 12 are the structural coordinates of a crystalline human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. These structural coordinates describe the location of atoms of the IL-13Ra1 polypeptide in relation to each other, the location of atoms in the human IL-13Rα1 polypeptide in relation to the atoms in human IL-13, the location of atoms in human IL-13 in relation to each other, the location of atoms in human IL-13 in relation to the atoms in the mAb13.2 Fab fragment and the location of atoms in the mAb13.2 Fab fragment in relation to each other.

The structural coordinates of a crystal can be modified by mathematical manipulation, such as by inversion or integer additions or subtractions. As such, structural coordinates are relative coordinates. As an example, structural coordinates describing the location of atoms in the mAb13.2 Fab fragment are not specifically limited by the actual x, y, and z coordinates of Table 10. As another example, structural coordinates describing the location of atoms in the human IL-13 bound to the mAb13.2 Fab fragment are not specifically limited by the actual x, y, and z coordinates of Table 11. As yet another example, structural coordinates describing the location of atoms in the human IL-13 bound to both the mAb13.2 Fab fragment and

the human IL-13R α 1 polypeptide are not specifically limited by the actual x, y, and z coordinates of Table 12.

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The structural coordinates of the mAb13.2 Fab fragment or human IL-13/mAb13.2 Fab fragment complex or human IL-Ra1 polypeptide/human IL-13/mAb 13.2 Fab fragment complex can be used to derive a representation (e.g., a two dimensional representation or three dimensional representation) of the mAb13.2 Fab fragment, a fragment of the mAb13.2 Fab fragment, human IL-13, a fragment of human IL-13, the human IL-13Rα1 polypeptide, a fragment of the IL-13Rα1 polypeptide, the human IL-13/mAb13.2 Fab fragment complex or human IL-Rα1 polypeptide/human IL-13/mAb 13.2 Fab fragment complex, or a fragment of either complex. Such a representation can be useful for a number of applications, including, for example, the visualization, identification and characterization of an active site of the polypeptide. In certain embodiments, a three-dimensional representation can include the structural coordinates of the mAb13.2 fragment according to Table 10 \pm a root mean square deviation from the alpha carbon atoms of amino acids of about 1.5 Å or less (e.g., about 1.0 Å or less, or about 0.5 Å or less). In other embodiments, a three-dimensional representation can include the structural coordinates of a human IL-13/mAb13.2 Fab fragment complex according to Table 11 ± a root mean square deviation from the alpha carbon atoms of amino acids of not more than about 1.5 Å (e.g., not more than about 1.0 Å, not more than about 0.5 Å or less). In yet other embodiments, a three-dimensional representation can include the structural coordinates of a human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex according to Table 12 ± a root mean square deviation from the alpha carbon atoms of amino acids of not more than about 1.5 Å (e.g., not more than about 1.0 Å, not more than about 0.5 Å or less). Root mean square deviation (rms deviation, or rmsd) is the square root of the arithmetic mean of the squares of the deviations from the mean, and is a way of expressing deviation or variation from structural coordinates. Conservative substitutions of amino acids can result in a molecular representation having structural coordinates within the stated root mean square deviation. For example, two molecular models of polypeptides that differ from one another by conservative amino acid substitutions can have coordinates of backbone atoms within a stated rms deviation, such as less than about 1.5 Å (e.g., less than about about 1.0 Å, less than about 0.5 Å). Backbone atoms of a polypeptide include

the alpha carbon (C_{α} or CA) atoms, carbonyl carbon (C) atoms, and amide nitrogen (N) atoms.

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Various software programs allow for the graphical representation of a set of structural coordinates to obtain a representation of a molecule or molecular complex, such as the mAb13.2 Fab fragment or the human IL-13/mAb13.2 Fab fragment complex or the human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. In general, such a representation should accurately reflect (relatively and/or absolutely) structural coordinates, or information derived from structural coordinates, such as distances or angles between features. The representation can be a twodimensional figure, such as a stereoscopic two-dimensional figure, or an interactive two-dimensional display (e.g., a computer display that can display different faces of the molecule or molecular complex), or an interactive stereoscopic two-dimensional display. An interactive two-dimensional display can be, for example, a computer display that can be rotated to show different faces of a polypeptide, a fragment of a polypeptide, a complex and/or a fragment of a complex. In some embodiments, the representation is a three-dimensional representation. As an example, a threedimensional model can be a physical model of a molecular structure (e.g., a ball-andstick model). As another example, a three dimensional representation can be a graphical representation of a molecular structure (e.g., a drawing or a figure presented on a computer display). A two-dimensional graphical representation (e.g., a drawing) can correspond to a three-dimensional representation when the two-dimensional representation reflects three-dimensional information, for example, through the use of perspective, shading, or the obstruction of features more distant from the viewer by features closer to the viewer. In some embodiments, a representation can be modeled at more than one level. As an example, when the three-dimensional representation includes a polypeptide, such as human IL-13 bound to the mAb13.2 Fab fragment, the polypeptide can be represented at one or more different levels of structure, such as primary structure (amino acid sequence), secondary structure (e.g., α-helices and βsheets), tertiary structure (overall fold), and quaternary structure (oligomerization state). The heavy and light chain polypeptides of the mAb13.2 Fab fragment can also be represented at the one or more different structural levels. A representation can include different levels of detail. For example, the representation can include the relative locations of secondary structural features of a protein without specifying the

positions of atoms. A more detailed representation could, for example, include the positions of atoms.

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In some embodiments, a representation can include information in addition to the structural coordinates of the atoms in the mAb13.2 Fab fragment, the human IL-13/mAb13.2 Fab fragment complex, or the human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. For example, a representation can provide information regarding the shape of a solvent accessible surface, the van der Waals radii of the atoms of the model, and the van der Waals radius of a solvent (e.g., water). Other features that can be derived from a representation include, for example, electrostatic potential, the location of voids or pockets within a macromolecular structure, and the location of hydrogen bonds and salt bridges.

An agent that interacts with the mAb13.2 Fab fragment, human IL-13, or the human IL-13Rα1 polypeptide can be identified or designed by a method that includes using a representation of the mAb13.2 Fab fragment, a human IL-13, a human IL-13Rα1 polypeptide, a human IL-13/mAb13.2 Fab fragment complex, or a human IL-13-Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. Exemplary types of representations include the representations discussed above. In some embodiments, the representation can be of an analog polypeptide, polypeptide fragment, complex or fragment of a complex. A candidate agent that interacts with the representation can be designed or identified by performing computer fitting analysis of the candidate agent with the representation. In general, an agent is a molecule. Examples of agents include polypeptides, nucleic acids (including DNA or RNA), or small molecules (e.g., small organic molecules). An agent can be a ligand, and can act, for example, as an agonist or antagonist. An agent that interacts with a polypeptide (e.g., human IL-13, human IL-13Rα1 polypeptide) can interact transiently or stably with the polypeptide. The interaction can be mediated by any of the forces noted herein, including, for example, hydrogen bonding, electrostatic forces, hydrophobic interactions, and van der Waals interactions.

As noted above, X-ray crystallography can be used to obtain structural coordinates of an mAb13.2 Fab fragment, a human IL-13/mAb13.2 Fab fragment complex, or a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. However, such structural coordinates can be obtained using other techniques including NMR techniques. Additional structural information can be

obtained from spectral techniques (e.g., optical rotary dispersion (ORD), circular dichroism (CD)), homology modeling, and computational methods such as those that include data from molecular mechanics or from dynamics assays).

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In some embodiments, the X-ray diffraction data can be used to construct an electron density map of the mAb13.2 Fab fragment, the human IL-13/mAb13.2 Fab fragment complex, or the human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex. The electron density map can be used to derive a representation (e.g., a two dimensional representation or a three dimensional representation) of the mAb13.2 Fab fragment, a fragment of the mAb13.2 Fab fragment, human IL-13 or a fragment of human IL-13, the human IL-13Rα1 polypeptide or a fragment of the human IL-13Ra1 polypeptide, the human IL-13/mAb13.2 Fab fragment complex, the human IL-13Ra1 polypeptide/human IL-13/mAb13.2 Fab fragment complex, or a fragment of either complex. Creation of an electron density map typically involves using information regarding the phase of the X-ray scatter. Phase information can be extracted, for example, either from the diffraction data or from supplementing diffraction experiments to complete the construction of the electron density map. Methods for calculating phase from X-ray diffraction data include, without limitation, multiwavelength anomalous dispersion (MAD), multiple isomorphous replacement (MIR), multiple isomorphous replacement with anomalous scattering (MIRAS), single isomorphous replacement with anomalous scattering (SIRAS), reciprocal space solvent flattening, molecular replacement, or a combination thereof. These methods generate phase information by making isomorphous structural modifications to the native protein, such as by including a heavy atom or changing the scattering strength of a heavy atom already present, and then measuring the diffraction amplitudes for the native protein and each of the modified cases. If the position of the additional heavy atom or the change in its scattering strength is known, then the phase of each diffracted X-ray can be determined by solving a set of simultaneous phase equations. The location of heavy atom sites can be identified using a computer program, such as SHELXS (Sheldrick, Institut Anorg. Chemie, Göttingen, Germany), and diffraction data can be processed using computer programs such as MOSFLM, SCALA, SOLOMON, and SHARP ("The CCP4 Suite: Programs for Protein Crystallography," Acta Crystallogr. Sect. D, 54:905-921, 1997; deLa Fortelle and Brigogne, Meth.

Enzym. 276:472-494, 1997). Upon determination of the phase, an electron density map of the complex can be constructed.

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The electron density map can be used to derive a representation of a polypeptide, a complex, or a fragment of a polypeptide or complex by aligning a three-dimensional model of a polypeptide or complex (e.g., a complex containing a polypeptide bound to an antibody) with the electron density map. The alignment process results in a comparative model that shows the degree to which the calculated electron density map varies from the model of the previously known polypeptide or the previously known complex. The comparative model is then refined over one or more cycles (e.g., two cycles, three cycles, four cycles, five cycles, six cycles, seven cycles, eight cycles, nine cycles, ten cycles) to generate a better fit with the electron density map. A software program such as CNS (Brunger et al., Acta Crystallogr. <u>D54</u>:905-921, 1998) can be used to refine the model. The quality of fit in the comparative model can be measured by, for example, an R_{work} or R_{free} value. A smaller value of R_{work} or R_{free} generally indicates a better fit. Misalignments in the comparative model can be adjusted to provide a modified comparative model and a lower R_{work} or R_{free} value. The adjustments can be based on information relating to human IL-13, human IL-13Rα1, the mAb13.2 Fab fragment, the previously known polypeptide and/or the previously known complex. Such information includes, for example, estimated helical or beta sheet content, hydrophobic and hydrophilic domains, and protein folding patterns, which can be derived, for example, from amino acid sequence, homology modeling, and spectral data. As an example, in embodiments in which a model of a previously known complex of a polypeptide bound to a ligand is used, an adjustment can include replacing the ligand in the previously known complex with the mAb13.2 fragment. As another example, in certain embodiments, an adjustment can include replacing an amino acid in the previously known polypeptide with the amino acid in the corresponding site of human IL-13. When adjustments to the modified comparative model satisfy a best fit to the electron density map, the resulting model is that which is determined to describe the antibody or polypeptide or complex from which the X-ray data was derived (e.g., the human IL-13/mAb13.2 Fab fragment complex). Methods of such processes are disclosed, for example, in Carter and Sweet, eds., "Macromolecular Crystallography" in Methods in Enzymology, Vol. 277, Part B, New York: Academic Press, 1997, and

articles therein, e.g., Jones and Kjeldgaard, "Electron-Density Map Interpretation," p. 173, and Kleywegt and Jones, "Model Building and Refinement Practice," p. 208.

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In some embodiments, a representation of the mAb13.2 Fab fragment can be derived by aligning a previously determined structural model of a different (but similar) antibody Fab fragment (e.g., a 2E8 Fab antibody fragment, Protein Databank Identification No. 12E8) with the electron density map of the mAb13.2 Fab fragment derived from X-ray diffraction data. A representation of a human IL-13/mAb13.2 Fab fragment complex can subsequently be derived by aligning the previously determined structural model of the mAb13.2 Fab fragment with the electron density map of the complex. A representation of a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex can subsequently be derived by aligning the previously determined structural model of the human IL-13/mAb13.2 Fab fragment complex with the electron density map of the human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex

A machine, such as a computer, can be programmed in memory with the structural coordinates of the mAb13.2 Fab fragment, a human IL-13/mAb13.2 Fab fragment complex, or a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 Fab fragment complex together with a program capable of generating a three-dimensional graphical representation of the structural coordinates on a display connected to the machine. Alternatively or additionally, a software system can be designed and/or utilized to accept and store the structural coordinates. The software system can be capable of generating a graphical representation of the structural coordinates. The software system can also be capable of accessing external databases to identify compounds (e.g., polypeptides) with similar structural features as human IL-13 or human IL-13Rα1, and/or to identify one or more candidate agents with characteristics that may render the candidate agent(s) likely to interact with human IL-13 or human IL-13Rα1. The software system can also be capable of accessing external databases to identify compounds that interact with human IL-13 or human IL-13Rα1 by virtue of the knowledge of the structure of the mAb13.2 Fab fragment, or human IL-13Rα1 polypeptide, and its interaction with human IL-13.

A machine having a memory containing structure data or a software system containing such data can aid in the rational design or selection of IL-13 ligands, such as agonists or antagonists. For example, such a machine or software system can aid in

the evaluation of the ability of an agent to associate with human IL-13, can aid in the modeling of compounds or proteins related by structural or sequence homology to human IL-13, or can aid in the evaluation of the ability of an agent to interfere with the bioactivity of human IL-13. A bioactivity of human IL-13can be any effect that the polypeptide elicits on or in a cell or tissue *in vivo* or *in vitro*. Exemplary bioactivities of human IL-13 are described herein, such as in Examples 1 and 2.

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A machine having a memory containing structure data or a software system containing such data can aid in the rational design or selection of IL-13R α 1 ligands, such as agonists or antagonists. For example, such a machine or software system can aid in the evaluation of the ability of an agent to associate with a human IL-13R α 1 polypeptide, can aid in the modeling of compounds or proteins related by structural or sequence homology to a human IL-13R α 1 polypeptide, or can aid in the evaluation of the ability of an agent to interfere with the bioactivity of a human IL-13R α 1 polypeptide. A bioactivity of a human IL-13R α 1 polypeptide can be any affect that the polypeptide elicits on or in a cell or tissue *in vivo* or *in vit*ro. Exemplary bioactivities of human IL-13R α 1 are described herein, such as in Example 3.

The machine can produce a representation (e.g., a two dimensional representation or a three dimensional representation) of the mAb13.2 Fab fragment or a fragment of the mAb13.2 Fab fragment, human IL-13 or a fragment of human IL-13, a human IL-13Rα1 polypeptide or a fragment of a human IL-13Rα1 polypeptide, a human IL-13/mAb13.2 Fab fragment complex, a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 fab fragment complex, or a fragment of either complex. A software system, for example, can cause the machine to produce such information. The machine can include a machine-readable data storage medium including a data storage material encoded with machine-readable data. The machinereadable data can include structural coordinates of atoms of the mAb13.2 Fab fragment or atoms of a fragment of the mAb13.2 Fab fragment, atoms of human IL-13 or atoms of a fragment of human IL-13, atoms of a human IL-13/mAb13.2 Fab fragment complex, atoms of a human IL-13Ra1 polypeptide/human IL-13/mAb13.2 fab fragment complex, or atoms of either complex. Machine-readable storage media including data storage material can include conventional computer hard drives, floppy disks, DAT tape, CD-ROM, DVD, and other magnetic, magneto-optical, optical, and other media which may be adapted for use with a computer. The machine can also

have a working memory for storing instructions for processing the machine-readable data, as well as a central processing unit (CPU) coupled to the working memory and to the machine-readable data storage medium for the purpose of processing the machine-readable data into the desired three-dimensional representation. Finally, a display can be connected to the CPU so that the three-dimensional representation may be visualized by the user. Accordingly, when used with a machine programmed with instructions for using the data (e.g., a computer loaded with one or more programs of the sort described herein) the machine is capable of displaying a graphical representation (e.g., a two dimensional graphical representation, a three-dimensional graphical representation) of any of the polypeptides, polypeptide fragments, complexes, or complex fragments described herein.

A display (e.g., a computer display) can show a representation of the mAb13.2 Fab fragment or a fragment of the mAb13.2 Fab fragment, human IL-13 or a fragment of human IL-13, a human IL-13Rα1 polypeptide or a fragment of a human IL-13Rα1 polypeptide, a human IL-13/mAb13.2 Fab fragment complex, a human IL-13Rα1 polypeptide/human IL-13/mAb13.2 fab fragment complex, or a fragment of either complex. The representation can also include an agent bound to human IL-13 or the human IL-13Rα1 polypeptide, or the user can superimpose a three-dimensional model of an agent on the representation of human IL-13 or the human IL-13Rα1 polypeptide. The agent can be an agonist (e.g., a candidate agonist) of human IL-13 or human IL-13Rα1, or an antagonist (e.g., a candidate antagonist) of human IL-13 or human IL-13Rα1. In some embodiments, the agent can be a known compound or fragment of a compound. In certain embodiments, the agent can be a previously unknown compound, or a fragment of a previously unknown compound.

The user can inspect the resulting representation. A representation of the mAb13.2 Fab fragment or fragment of the mAb13.2 Fab fragment, human IL-13 or fragment of the human IL-13, the human IL-13Ra1 polypeptide or fragment of the human IL-13Ra1 polypeptide, the human IL-13/mAb13.2 Fab fragment complex, the human IL-13Ra1 polypeptide/human IL-13/mAb13.2 fab fragment complex, or the fragment of either complex can be generated, for example, by altering a previously existing representation of such polypeptides and polypeptide complexes. For example, there can be a preferred distance, or range of distances, between atoms of the antibody and atoms of the human IL-13 when considering a new representation of

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a complex or fragment of a complex. In another example, there can be a preferred distance, or range of distances, between atoms of the human IL-13 and the human IL-13Rα1 polypeptide when considering a new representation of a complex or fragment of a complex. Distances longer than a preferred distance may be associated with a weak interaction between the agent and active site (e.g., the site of IL-13 receptor binding (such as to an IL-13Ra1 receptor polypeptide or an IL-4 receptor polypeptide) on the IL-13 polypeptide). Distances shorter than a preferred distance may be associated with repulsive forces that can weaken the interaction between the agent and the polypeptide. A steric clash can occur when distances between atoms are too short. A steric clash occurs when the locations of two atoms are unreasonably close together, for example, when two atoms are separated by a distance less than the sum of their van der Waals radii. If a steric clash exists, the user can adjust the position of the agent relative to the human IL-13 (e.g., a rigid body translation or rotation of the agent), until the steric clash is relieved. The user can adjust the conformation of the agent or of the human IL-13 in the vicinity of the agent in order to relieve a steric clash. Steric clashes can also be removed by altering the structure of the agent, for example, by changing a "bulky group," such as an aromatic ring, to a smaller group, such as to a methyl or hydroxyl group, or by changing a rigid group to a flexible group that can accommodate a conformation that does not produce a steric clash. Electrostatic forces can also influence an interaction between an agent and a polypeptide (such as the part of the polypeptide that interacts with a receptor polypeptide, e.g., a human IL-13Rα1 polypeptide or a human IL-4R polypeptide). For example, electrostatic properties can be associated with repulsive forces that can weaken the interaction between the agent and the IL-13 polypeptide. Altering the charge of the agent, e.g., by replacing a positively charged group with a neutral group can relieve electrostatic repulsion. Similar processes can be performed to design an agent that interacts with a human IL-13Rα1 polypeptide, such as in the vicinity of interaction between the human IL-13Rα1 polypeptide and human IL-13.

Forces that influence binding strength between the mAb13.2 Fab fragment and human IL-13 can be evaluated in the polypeptide/agent model. Likewise, forces that influence binding strength between human IL-13 and the human IL-13R α 1 polypeptide can be evaluated in the polypeptide/agent model. These can include, for example, hydrogen bonding, electrostatic forces, hydrophobic interactions, van der

Waals interactions, dipole-dipole interactions, π-stacking forces, and anion-π interactions. The user can evaluate these forces visually, for example by noting a hydrogen bond donor/acceptor pair arranged with a distance and angle suitable for a hydrogen bond. Based on the evaluation, the user can alter the model to find a more favorable interaction between the human IL-13, or human IL-13Rα1 polypeptide, and the agent. Altering the model can include changing the three-dimensional structure of the polypeptide without altering its chemical structure, for example by altering the conformation of amino acid side chains or backbone dihedral angles. Altering the model can include altering the position or conformation of the agent, as described above. Altering the model can also include altering the chemical structure of the agent, for example by substituting, adding, or removing groups. For example, if a hydrogen bond donor on the human IL-13 is located near a hydrogen bond donor on the agent, the user can replace the hydrogen bond donor on the agent with a hydrogen bond acceptor.

The relative locations of the agent and the human IL-13, or their conformations, can be adjusted to find an optimized binding geometry for a particular agent to the IL-13 polypeptide. Likewise, the relative locations of the agent and the human IL-13Rα1 polypeptide can be adjusted to find an optimized binding geometry for a particular agent to the human IL-13Rα1 polypeptide. An optimized binding geometry is characterized by, for example, favorable hydrogen bond distances and angles, maximal electrostatic attractions, minimal electrostatic repulsions, the sequestration of hydrophobic moieties away from an aqueous environment, and the absence of steric clashes. The optimized geometry can have the lowest calculated energy of a family of possible geometries for a human IL-13 /antibody complex, or a human IL-13/receptor complex. An optimized geometry can be determined, for example, through molecular mechanics or molecular dynamics calculations.

A series of representations of human IL-13 bound to different agents can be generated. Likewise, a series of representations of a human IL-13Rα1 polypeptide bound to different agents can be generated. A score can be calculated for each representation. The score can describe, for example, an expected strength of interaction between human IL-13 and the agent. The score can reflect one of the factors described above that influence binding strength. The score can be an

aggregate score that reflects more than one of the factors. The different agents can be ranked according to their scores.

Steps in the design of the agent can be carried out in an automated fashion by a machine (e.g., a computer). For example, a representation of human IL-13, or a human IL-13Ra1 polypeptide can be programmed in the machine, along with representations of candidate agents. The machine can find an optimized binding geometry for each of the candidate agents to the site of receptor binding, and calculate a score to determine which of the agents in the series is likely to interact most strongly with human IL-13, or the human IL-13Ra1 polypeptide.

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A software system can be designed and/or implemented to facilitate these steps. Software systems (e.g., computer programs) used to generate representations or perform the necessary fitting analyses include, but are not limited to: MCSS, Ludi, QUANTA, Insight II, Cerius2, CHARMm, and Modeler from Accelrys, Inc. (San Diego, CA); SYBYL, Unity, FleXX, and LEAPFROG from TRIPOS, Inc. (St. Louis, MO); AUTODOCK (Scripps Research Institute, La Jolla, CA), GRID (Oxford University, Oxford, UK); DOCK (University of California, San Francisco, CA); and Flo⁺ and Flo99 (Thistlesoft, Morris Township, NJ). Other useful programs include ROCS, ZAP, FRED, Vida, and Szybki from Openeye Scientific Software (Santa Fe, NM); Maestro, Macromodel, and Glide from Schrodinger, LLC (Portland, OR); MOE (Chemical Computing Group, Montreal, Quebec), Allegrow (Boston De Novo, Boston, MA), CNS (Brunger, et al., Acta Crystall. Sect. D 54:905-921, 1997) and GOLD (Jones et al., J. Mol. Biol. 245:43-53, 1995. The structural coordinates can also be used to visualize the three-dimensional structure of human IL-13 using MOLSCRIPT, RASTER3D, or PYMOL (Kraulis, J. Appl. Crystallogr. 24: 946-950, 1991; Bacon and Anderson, J. Mol. Graph. 6: 219-220, 1998; DeLano, The PYMOL Molecular Graphics System (2002) DeLano Scientific, San Carlos, CA).

The agent can, for example, be selected by screening an appropriate database, can be designed *de novo* by analyzing the steric configurations and charge potentials of an unbound human IL-13, or unbound human IL-13Rα1 polypeptide, in conjunction with the appropriate software systems, and/or can be designed using characteristics of known cytokine ligands. The agent can be tested for an ability to block binding of IL-13 to an IL-4R polypeptide, such as IL-4Rα, or an IL-Rα1 polypeptide. An agent can be designed for binding to human IL-13 or to the human

IL-13Rα1 polypeptide. The method can be used to design or select agonists or antagonists of human IL-13 or a human IL-Rα1 polypeptide. A software system can be designed and/or implemented to facilitate database searching, and/or agent selection and design.

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Once an agent has been designed or identified, it can be obtained or synthesized and further evaluated for its affect on human IL-13 activity or on human IL-13R α 1 activity. The agent can be evaluated by contacting it with human IL-13 and assaying IL-13 bioactivity, or by contacting it with a human IL-13Ra1 polypeptide and assaying IL-13Ra1 bioactivity. A method for evaluating the agent can include an activity assay performed in vitro or in vivo. An activity assay can be a cell-based assay, for example. Depending upon the action of the agent on human IL-13 or the human IL-13Rα1 polypeptide, the agent can act either as an agonist or antagonist of human IL-13 or IL-13Rα1 activity. An agonist will cause human IL-13 or human IL-13Rα1 polypeptide to have the same or similar activity, and an antagonist will inhibit a normal function of human IL-13 or the human IL-13Rα1 polypeptide. An agent can be contacted with the human IL-13 in the presence of an anti-IL-13 antibody (e.g., mAb13.2 or mAb13.2 Fab) or a human IL-13 receptor (e.g., an IL-4R polypeptide, such as a human IL-4R α polypeptide, or an IL-13R polypeptide, such as a human IL-13Ra1 polypeptide) to determine whether or not the agent inhibits binding of the antibody or the receptor to the human IL-13 polypeptide. In some embodiments, the agent will inhibit binding of one kind of receptor to human IL-13, but will not inhibit binding of another kind of receptor. For example, an agent can inhibit binding of a human IL-13 polypeptide to a human IL-4R polypeptide (e.g., the IL-4R α chain), but not a human IL-13R α 1 polypeptide. Likewise, a different agent can inhibit binding of human IL-13 to an IL-13R α 1 polypeptide but not to a human IL-4R polypeptide. In another embodiment, the agent will inhibit binding of the IL-13 polypeptide to a human IL 4R polypeptide (e.g., the IL-4R α chain) and a human IL-13R α 1 polypeptide. A crystal containing human IL-13 bound to the identified agent can be grown and the structure determined by X-ray crystallography. A second agent can be designed or identified based on the interaction of the first agent with human IL-13. Various molecular analysis and rational drug design techniques are further disclosed in, for example, U.S. Patent Nos. 5,834,228, 5,939,528 and 5,856,116, as well as in PCT Application No. PCT/US98/16879, published as WO 99/09148.

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While certain embodiments have been described, other embodiments are also contemplated.

As an example, while embodiments involving human IL-13, the mAb13.2 Fab fragment, and a human IL-13Rα1 polypeptide have been described, more generally, any IL-13 polypeptide, any IL-13Rα1 polypeptide, and/or any anti-IL-13 antibody can be used.

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As an example, while embodiments have been described that involve human IL-13 and a human IL-13Rα1 polypeptide, more generally any IL-13 polypeptide and any IL-13Rα1 polypeptide can be used. For example, an IL-13 polypeptide or an IL-13Rα1 polypeptide can originate from a nonmammalian or mammalian species. Exemplary nonhuman mammals include, a nonhuman primate (such as a monkey or ape), a mouse, rat, goat, cow, bull, pig, horse, sheep, wild boar, sea otter, cat, or dog. Exemplary nonmammalian species include chicken, turkey, shrimp, alligator, or fish.

Further, an IL-13 polypeptide or an IL-13Rα1 polypeptide can generally be a full-length, mature polypeptide, including the full-length amino acid sequence of any isoform or processed form of an IL-13 polypeptide or IL-13Rα1 polypeptide. An isoform is any of several multiple forms of a protein that differ in their primary structure. Full-length IL-13 can be referred to as the precursor form of the protein. Full-length IL-13 has a signal peptide cleavage site. The IL-13 polypeptide can be the processed polypeptide, such as following cleavage of the signal peptide.

A human IL-13 polypeptide typically has at least one active site for interacting with a receptor polypeptide (e.g., an IL-4R polypeptide, an IL-13α1 polypeptide). An IL-13 polypeptide can include three active sites for interacting with two different receptor polypeptides. An anti-IL-13 antibody can be capable of binding to at least one of the active sites. In general, an active site can include a site of receptor polypeptide binding, or a site of phosphorylation, glycosylation, alkylation, acylation, or other covalent modification. An active site can include accessory binding sites adjacent or proximal to the actual site of binding that may affect activity upon interaction with the ligand. An active site of a human IL-13 polypeptide can include amino acids of SEQ ID NO:4. For example, an active site of a human IL-13 polypeptide can include one or more of amino acids Ser7, Thr8, Ala9, Glu12, Leu48, Glu49, Ile52, Asn53, Arg65, Ser68, Gly69, Phe70, Cys71, Pro72, His73, Lys74, and Arg86 as defined by the amino acid sequence of SEQ ID NO:4 (FIG. 2B). In some

embodiments, an agent can interact to within about 2.0Å or less (*e.g.*, about 1.5Å or less, about 1.0Å or less) of one or more amino acids Glu49, Asn53, Gly69, Pro72, His73, Lys74, and Arg86 of IL-13, as defined by the amino acid sequence of SEQ ID NO:4. In one alternative, an active site of a human IL-13 polypeptide can include one or more of amino acids Arg11, Glu12, Leu13, Ile14, Glu15, Lys104, Lys105, Leu106, Phe107, and Arg108 as defined by the amino acid sequence of SEQ ID NO:4. In another alternative, an active site of a human IL-13 polypeptide can include one or more of amino acids Thr88, Lys89, Ile90, and Glu91 as defined by the amino acid sequence of SEQ ID NO:4. A human IL-13 polypeptide can include one, two, or all three of the active sites described above.

A human IL-13Rα1 polypeptide typically has at least one active site for interacting with a polypeptide ligand (e.g., a human IL-13 polypeptide). An anti-IL-13Rα1 antibody can be capable of binding to at least one of the active sites. In general, an active site can include a site of polypeptide ligand binding, or a site of phosphorylation, glycosylation, alkylation, acylation, or other covalent modification. An active site can include accessory binding sites adjacent or proximal to the actual site of binding that may affect activity upon interaction with the ligand. An active site of a human IL-13Rα1 polypeptide can include amino acids of SEQ ID NO:12. For example, an active site of a human IL-13Rα1 polypeptide can include one or more of amino acid residues Ile254, Ser255, Arg256, Lys318, Cys320, and Tyr321 as defined by the amino acid sequence of SEQ ID NO:12. In one alternative, an active site of a human IL-13Rα1 polypeptide can include one or more of amino acid residues Lys76, Lys77, Ile78, and Ala79 as defined by the amino acid sequence of SEQ ID NO:12. A human IL-13Rα1 polypeptide can include one or both of these active sites.

The numbering of the amino acids of a human IL-13 polypeptide, a human IL-13Rα1 polypeptide, and the heavy and light chains of an anti-IL-13 antibody, such as mAb13.2 Fab, may be different than that set forth here, and may contain certain conservative amino acid substitutions, additions or deletions that yield the same three-dimensional structure as those defined by Table 10, ± an rmsd for backbone atoms of less than 1.5 Å, or by Table 11, ± an rmsd for backbone atoms of less than 1.5 Å, or by Table 12, ± an rmsd for backbone atoms of less than 1.5 Å. For example, the numbering of a human IL-13 processed polypeptide may be different than that set forth in FIG. 2B, and the sequence of the IL-13 may contain conservative amino acid

substitutions but yield the same structure as that defined by the coordinates of Table 11 and illustrated in FIG. 3 or the same structure as that defined by the coordinates of Table 12 and illustrated in FIGs. 15,16 and 17. Corresponding amino acids and conservative substitutions in other isoforms or analogs are easily identified by visual inspection of the relevant amino acid sequences or by using commercially available homology software programs (e.g., MODELLAR, MSI, San Diego, CA).

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An analog is a polypeptide having conservative amino acid substitutions. Conservative substitutions are amino acid substitutions that are functionally or structurally equivalent to the substituted amino acid. A conservative substitution can include switching one amino acid for another with similar polarity, or steric arrangement, or belonging to the same class (e.g., hydrophobic, acidic or basic) as the substituted amino acid. Conservative substitutions include substitutions having an inconsequential effect on the three-dimensional structure of an anti-IL-13 antibody or a human IL-13 polypeptide/anti-IL-13 antibody complex or a human IL-13Ra1 polypeptide/human IL-13 polypeptide/anti-IL-13 antibody complex with respect to identification and design of agents that interact with the polypeptide (e.g., an IL-13 polypeptide, an IL-13Ra1 polypeptide), as well as for molecular replacement analyses and/or for homology modeling.

While examples have been described in which an anti-IL-13 antibody is derived from a mouse, more generally any anti-IL-13 antibody can be used. For example, an anti-IL-13 antibody can originate from a human, mouse, rat, hamster, rabbit, goat, horse, or chicken.

As another example, while embodiments have been described in which an anti-IL-13 antibody is generated by a certain method, other methods may also be used. For example, an anti-IL-13 antibody can be generated by first preparing polyclonal antisera by immunization of female BALB/c mice with recombinant or native human IL-13. Sera can be screened for binding to human IL-13 by an assay such as ELISA. Splenocytes from a mouse demonstrating high serum antibody titers can be fused with a myeloma cell line, such as the P3X63_AG8.653 myeloma cell line (ATCC, Manassas, VA), and plated in selective media. Fusions can be isolated following multiple rounds of subcloning by limiting dilution and the fusions can be screened for the production of antibodies that have a binding affinity to human IL-13.

An anti-IL-13 antibody can be polyclonal or monoclonal. An antibody that binds IL-13 can be a fragment of an antibody, such as a Fab fragment.

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In general, intact antibodies, also known as immunoglobulins, are tetrameric glycosylated proteins composed of two light (L) chains of approximately 25 kDa each and two heavy (H) chains of approximately 50 kDa each. Each light chain is composed of an N-terminal variable (V) domain (VL) and a constant (C) domain (CL). Each heavy chain is composed of an N-terminal V domain (VH), three or four C domains (CHs), and a hinge region. The CH domain most proximal to VH is designated as CH1. The VH and VL domain consist of four regions of relatively conserved sequence called framework regions, which form a scaffold for three regions of hypervariable sequence (complementarity determining regions, CDRs). The CDRs contain most of the residues responsible for specific interactions with the antigen. CDRs are referred to as CDR1, CDR2, and CDR3. Accordingly, CDR constituents on the heavy chain are referred to as H1, H2, and H3, while CDR constituents on the light chain are referred to as L1, L2, and L3 (see Table 4, for example). The subunit structures and three-dimensional configurations of different classes of immunoglobulins are well known in the art. For a review of antibody structure, see Antibodies: A Laboratory Manual, Cold Spring Harbor Laboratory, eds. Harlow et al. (1988). The smallest antigen-binding fragment is the Fv (Fragment variable), which consists of the VH and VL domains. The Fab (fragment antigen binding) fragment consists of the VH-CH1 and VL-CL domains covalently linked by a disulfide bond between the constant regions.

Accordingly, in one aspect, this application features an antibody or an antigenbinding fragment thereof, that binds to and/or neutralizes, IL-13. The antibody or fragment thereof can also be a human, humanized, chimeric, or *in vitro*-generated antibody. In one embodiment, the anti-IL-13 antibody or fragment thereof is a humanized antibody. The antibody includes one or more CDRs that has a backbone conformation of a CDR described in Table 10 ± a root mean square deviation (RMSD) of not more than 1.5, 1.2, 1.1, or 1.0 Angstroms, Table 11 ± an RMSD of not more than 1.5, 1.2, 1.1, or 1.0 Angstroms, or Table 12 ± an RMSD of not more than 1.5, 1.2, 1.1, or 1.0 Angstroms. For example, one, two, or three of the CDRs of the light chain variable domain (e.g., particularly in CDR1, or in at least two CDRs, e.g., CDR1 and CDR3, CDR1 and CDR2, or in all three CDRs) have an RMSD of not

more than 1.5, 1.2, 1.1, or 1.0 Angstroms, relative to those structures. In one embodiment, the antibody or antigen binding fragment thereof includes a variable domain that, as a whole, has a backbone conformation of a CDR described in Table 10 ± a root mean square deviation (RMSD) of not more than 1.5, 1.2, 1.1, or 1.0 Angstroms, Table 11 ± an RMSD of not more than 1.5, 1.2, 1.1, or 1.0 Angstroms, or Table 12 ± an RMSD of not more than 1.5, 1.2, 1.1, or 1.0 Angstroms. The variable domain can also be at least at least 70%, 80%, 85%, 87%, 90%, 92%, 93%, 95%, 96%, 97%, 98%, or 99% identical to an antibody described herein, e.g., in the CDR region and/or framework regions. The antibody can be used, e.g., in a method of treatment described herein.

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Anti-IL-13 antibodies are disclosed, for example, in U.S. Provisional Patent Application No. 60/578,473, filed June 9, 2004, U.S. Provisional Patent Application No. 60/581,375 filed June 22, 2004, and U.S. Patent Application No. _____ [Attorney Docket: AM101493] (Kasaian *et al.*), filed on even date herewith, each of which is incorporated herein by reference.

The following examples are illustrative and are not intended as limiting.

EXAMPLES

Example 1. Generation and functional analysis of mAb13.2. To generate an antibody that recognizes IL-13, polyclonal antisera were prepared by immunization of female BALB/c mice with recombinant human IL-13 (R&D Systems, Minneapolis, MN). Sera were screened for binding to human IL-13 by ELISA. Splenocytes from a mouse demonstrating high serum antibody titers were fused with the P3X63_AG8.653 myeloma cell line (ATCC, Manassas, VA), and plated in selective media. Fusions were isolated with three rounds of subcloning by limiting dilution and screened for the production of antibodies that had a binding affinity to human IL-13. Three monoclonal antibodies were capable of binding IL-13 and neutralizing and/or inhibiting its bioactivity. The monoclonal antibody mAb13.2 (IgG1κ) was the subject of further analysis.

Several assays were performed to confirm that the murine monoclonal antibody mAb13.2 binds with high affinity and specificity to human IL-13. First, Biacore analysis confirmed that mAb13.2 had a rapid on-rate, slow off-rate, and high affinity for binding to human IL-13 (FIG. 4).

tested, including native IL-13 derived from cord blood T cells (FIG. 5). To perform the assays with recombinant human IL-13, ELISA plates were coated with anti-FLAG M2 antibody. The binding of recombinant FLAG-tagged human IL-13 was detected with biotinylated mAb13.2 and streptavidin-peroxidase. This binding could be competed with native human IL-13 isolated from mitogen activated, TH2-skewed, cord blood mononuclear cells and with recombinant human IL-13 (FIG. 5). Recombinant murine IL-13 could not compete for binding with mAb13.2. Unlabeled mAb13.2 and unlabeled mAb13.2 Fab were also able to compete for binding to the flag-tagged IL-13 with biotinylated mAb13.2 (FIG. 11A). The IL-13 specific nonneutralizing monoclonal antibody mAb13.8 could not compete with biotinylated mAb13.2 binding.

The ability of mAb13.2 to neutralize IL-13 bioactivity *in vitro* was confirmed using a TF1 bioassay, human peripheral blood monocytes, and human peripheral blood B cells. In the presence of suboptimal concentrations of IL-13, the proliferation of cells of the human erythroleukemic TF1 cell line can be made IL-13-dependent. The TF1 cell line was starved for cytokine, then exposed to a suboptimal concentration (3 ng/mL) of recombinant human IL-13 in the presence of varying concentrations of purified mouse mAb13.2 or the soluble inhibitor rhuIL-13Rα2. Cells were incubated for three days, and ³H-thymidine incorporation over the final four hours was determined by liquid scintillation counting. At suboptimal IL-13 concentrations (3 ng/mL), mAb13.2 caused a dose-dependant inhibition of TF1 proliferation (FIG. 6 and FIG. 12A). The IC₅₀ for this effect, 250 pM, is comparable to the IC₅₀ of rhuIL-13Rα2. The mAb13.2 Fab also inhibited CD23 expression human PBMCs.

Human PBMCs respond to IL-13 or IL-4 by increasing cell-surface expression of low affinity IgE receptor (CD23) in a dose-dependent manner (see FIG. 7A). Monocytes (CD11b⁺) were therefore used to confirm the ability of mAb13.2 to neutralize IL-13 bioactivity. CD11b⁺ monocytes were treated for 12 hours with 1 ng/mL recombinant human IL-13 (FIG. 7B) or IL-4 (FIG. 7C) in the presence of the indicated concentration of purified mouse mAb13.2. Cells were then harvested and stained with CyChrome-labeled anti-CD11b antibodies and PE-labeled anti-CD23 antibodies. Labeling was detected by flow cytometry. The mAb13.2 inhibited IL-13-

induced CD23 expression (FIG. 7B; see also FIG. 12B), but did not inhibit IL-4-induced CD23 expression (FIG. 7C).

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The effects of mAb13.2 were also tested in a model of IL-13-induced IgE production by human peripheral blood B cells. In response to IL-13 and the T cell mitogen, phytohemaglutinin (PHA), human B cells undergo an Ig isotype switch recombination to IgE, resulting in higher IgE levels in culture. This effect can be seen as an increased frequency of IgE-producing B cells. To examine the effect of mAb13.2 on IL-13-dependent IgE production in B cells, PBMCs from a healthy donor were cultured in microtiter wells in the presence of autologous irradiated PBMC as feeders, and stimulated with PHA and IL-13. After 3 weeks, each well was assayed for IgE by ELISA. PHA + IL-13 increased the frequency of IgE-producing B cell clones. This effect was inhibited by mAb13.2, but not by mAb13.8 (binds IL-13 but does not neutralize), or by irrelevant mouse IgG:mAb13.2 efficiently blocked this effect of IL-13 on cultured B cells (FIG. 8).

Finally, the ability of mAb13.2 to block an early cellular response to IL-13 was tested by examining effects on signal transducer and activator of transcription (STAT) 6 phosphorylation. Upon IL-13 interaction with its cell surface receptor, STAT6 dimerizes, becomes phosphorylated, and translocates from the cytoplasm to the nucleus, where it activates transcription of cytokine-responsive genes (Murata et al., J. Biol. Chem. 270:30829-36, 1995). Specific antibodies against phosphorylated STAT6 can detect this activation by Western blot or flow cytometry within 30 min of IL-13 exposure. To test the effect of mAb13.2 on IL-13 dependent STAT6 phosphorylation, cells of the HT-29 human epithelial cell line were treated with the indicated concentration of IL-13 for 30 minutes at 37°C. Phospho-STAT6 was detected in cell lysates by Western blot (FIG. 9A) or by flow cytometry (FIGs. 9B and 9C). In the experiment illustrated in FIG. 9B, cells were treated with a saturating concentration of IL-13 for 30 minutes at 37°C and then fixed, permeabilized, and stained with an Alexa-Fluor 488-labeled mAb against phospho-STAT6. In the experiment illustrated in FIG. 9C, cells were treated with a suboptimal concentration of IL-13 in the presence or absence of an antibody, fixed and stained as described above. Flow cytometry results revealed that mAb13.2 blocked STAT6 phosphorylation, whereas mAb13.8 and the control mouse IgG1 had no effect.

Example 2: Murine monoclonal antibody mAb13.2 neutralizes IL-13 bioactivity in vivo. The ability of mouse mAb13.2 to neutralize IL-13 activity in vivo was tested using a model of antigen-induced airway inflammation in Cynomolgus monkeys naturally allergic to Ascaris suum. In this model, challenge of an allergic monkey with Ascaris suum antigen results in an influx of inflammatory cells, especially eosinophils, into the airways. To test the ability of mAb13.2 to prevent this influx of cells, the antibody was administered 24 hours prior to challenge with Ascaris suum antigen. On the day of challenge, a baseline lavage sample was taken from the left lung. The antigen was then instilled intratracheally into the right lung. Twentyfour hours later, the right lung was lavaged, and the bronchial alveolar lavage (BAL) fluid from animals treated intravenously with 8 mg/kg ascites purified mAb13.2 were compared to BAL fluid from untreated animals. Eosinophil counts increased in 4 of 5 untreated animals following challenge, as compared to 1 of 6 animals treated with mAb13.2 (FIG. 10). The percent BAL eosinophils was significantly increased for the untreated group (p<0.02), but not for the antibody-treated group. These results confirmed that mAb13.2 effectively prevents airway eosinophilia in allergic animals challenged with an allergen.

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The average serum half-life of mouse mAb13.2 was less than one week in the monkeys. At the 3-month time point, when all traces of mAb13.2 would have been gone from the serum, mAb13.2-treated animals were rechallenged with *Ascaris suum* to confirm the *Ascaris* responsiveness of those individuals. Two of six monkeys in the treated group were found to be nonresponders.

Example 3: Murine monoclonal antibody mAb13.2 binds to a region of IL-13 that normally binds to IL-4Rα. IL-13 bioactivity is mediated through a receptor complex consisting of the IL-13Rα1 and IL-4Rα chains. The cytokine first undergoes a relatively low affinity interaction with IL-13Rα1 on the surface of cells. This complex then recruits IL-4Rα to form the high affinity receptor (Zurawski *et al.*, *EMBO J.* 12:2663, 1993; Zurawski *et al.*, *J. Biol. Chem.* 270:23869, 1995). Signaling through the IL-4Rα chain involves phosphorylation of STAT6, which can be monitored as one of the earliest cellular responses to IL-13 (Murata *et al.*, *J. Biol. Chem.* 270:30829-36, 1995). Several approaches, such as epitope mapping, X-ray crystallography, and further Biacore analysis, were used to elucidate the interaction

between murine mAb13.2 antibody and human IL-13, and further determine the basis for the IL-13 neutralizing effects of this antibody.

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Epitope mapping and X-ray crystallography analysis indicated that mAb13.2 binds to the C-terminal region of IL-13 helix C, i.e., the IL-4R binding region (see below). To confirm this analysis, the interaction between mAb13.2 and IL-13 was analyzed with a Biacore chip. This analysis was done in several formats. First, IL-4R was bound to the Biacore chip, and a complex of IL-13 prebound to IL-13Rα1 was flowed over the chip. In the absence of mAb13.2, formation of a tri-molecular complex could be demonstrated. However, addition of mAb13.2 to the mixture of IL-13 prebound to IL-13Rα1 prevented binding to IL-4R on the chip. Second, mAb13.2 was immobilized on the chip and bound IL-13 was added in solution phase. Although IL-13Rα1 was found to interact with the bound IL-13, no interaction of IL-4R with bound IL-13 was detected. Third, it was demonstrated that mAb13.2 could bind to IL-13 that was bound to IL-13Rα1-Fc or IL-13Rα1 monomer immobilized on the chip. These observations indicate that mAb13.2 does not inhibit IL-13 interaction with IL-13Rα1 but disrupts the interaction of IL-13Rα1 with IL-4Rα. This disruption is thought to prevent formation of the IL-13 signaling complex. These observations provided a model for the neutralization activity of this antibody.

The *in vitro* demonstration of a complex of mAb13.2 with IL-13 and IL-13Ra1 suggests that mAb13.2 could potentially be bound to receptor-associated IL-13 at the cell surface. In order to determine whether cell-bound mAb13.2 could be detected under conditions of saturating receptor-bound IL-13, the HT-29 human epithelial cell line was loaded with IL-13 at 4°C and tested for antibody binding. No cell-bound mAb could be detected by flow cytometry. This observation, together with the demonstration that mAb13.2 is a potent neutralizer of IL-13 bioactivity, indicated that normal functioning of the IL-13 receptor is disrupted by mAb13.2.

Example 4: Crystal structure of anti-IL-13 antibody mAb13.2 Fab fragment. Monoclonal antibody mAb13.2 from mouse ascites was purified using a Protein A affinity column. The mouse ascites was diluted 2X with Protein A binding buffer (50mM Tris-HCl, 500mM NaCl, pH 8.0) and filtered through a 0.2 mm filter unit. The filtered solution was applied to a Poros Protein A column (Applied Biosystems, Framingham, MA) equilibrated with the binding buffer at 4°C. The column was

washed with the binding buffer, and the IgG was eluted using 100 mM Glycine (pH 3.0). The eluted IgG was neutralized immediately with 1M Tris-HCl at pH 8.0.

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The Fab fragment was prepared by digesting the IL-13 monoclonal IgG with activated papain (Sigma, St. Louis, MO). Papain was activated by diluting the stock enzyme solution with the digestion buffer (50mM Tris-HCl, 50mM NaCl, 20mM EDTA and 20 mM Cysteine, pH 7.5) on ice to give a final papain concentration of 1mg/mL. Cleavage of IgG was performed by incubation with activated papain at a ratio of 100:1 w/w in papain digestion buffer for 7-8 hours at 37°C. The reaction was stopped by dialysis in 50 mM Tris-HCl (pH 7.5) overnight at 4°C. The dialyzed solution was loaded onto a tandem Poros HS/Protein A column equilibrated with 50 mM Tris-HCl (pH 7.5) at 4°C to remove the papain and the Fc fragment. The flowthrough of the tandem columns containing the Fab fragment was then loaded onto a hydroxylapatite column (Bio-Rad, Hercules, CA) equilibrated with 1 mM Sodium Phosphate and 20 mM Tris-HCl, pH 7.5, and eluted with a 1 mM to 125 mM Sodium Phosphate gradient at 25°C. The eluted Fab fragment solution was dialyzed overnight in 50 mM Tris-HCl (pH 8.0) at 4°C. After dialysis, the solution was loaded onto a Poros HQ column equilibrated with 50 mM Tris-HCl (pH 8.0). The flow-through was collected and ammonium sulfate was adjusted to a final concentration of 1.5 M before loading onto a Polypropyl Aspartamide column (Nest Group, Southborough, MA). The Fab fragment was eluted from the column with a 1.5 to 0 M ammonium sulfate gradient at 25°C. The protein was dialyzed in 50 mM Tris-HCl (pH 8.0) at 4°C.

The isolated mAb13.2 antibody and mAb13.2 Fab fragment were tested for their ability to inhibit IL-13 bioactivity. In one assay, purified mAb13.2 and mAb13.2 Fab fragment were tested for their ability to compete for binding with biotinylated mAb13.2 in an ELISA assay. ELISA plates were coated with anti-FLAG M2 antibody. The binding of FLAG-human IL-13 was detected with biotinylated mAb13.2 and streptavidin-peroxidase. Both the intact antibody and the Fab fragment were able to compete for binding, while the IL-13-specific nonneutralizing antibody mAb13.8 could not compete for binding (FIGs. 11A and 11B).

In other assays, purified mAb13.2 and mAb13.2 Fab fragment were tested for their ability to inhibit IL-13-dependent TF1 cell proliferation and IL-13-dependent CD23 expression on PBMCs. TF1 cells were incubated with 3 ng/mL recombinant human IL-13 as described in Example 1. The cells were treated with increasing

concentrations of purified mAb13.2 or mAb13.2 Fab, and cell proliferation was monitored as described. Both the intact antibody and the Fab fragment inhibited IL-13-dependent TF1 cell proliferation (FIG. 12A). To test the effect of the isolated proteins on CD23 expression, PBMCs were incubated with 1 ng/mL recombinant human IL-13 as described in Example 1. The monocytes were treated with increasing concentrations of mAb13.2 or mAb13.2 Fab, and CD23 expression was monitored by flow cytometry as described above. The purified intact antibody and the purified Fab fragment were each capable of inhibiting IL-13-dependent CD23 expression (FIG. 12B).

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For crystallization, purified mAb13.2 Fab was prepared at a concentration of 12.6 mg/mL in a solution of 50 mM Tris (pH 8.0) and 50 mM NaCl. One microliter of protein solution was mixed with 1 μ l of crystallization solution (20% PEG 3350, 200 mM K₂SO₄) (Hampton Research, Aliso Viejo, CA), and the crystals formed at about 18° C by the hanging drop method of vapor diffusion.

Data from crystals for the mAb13.2 Fab fragment were collected on beamline 5.0.2 at the Advanced Light Source (ALS) (Berkley, CA) using an ADSC Quantum-4 CCD detector. A single crystal, vitrified at -180°C, was used for each data set. The data were processed using DENZO and Scalepack (Otwinowski and Minor, *Methods Enzymol.* 276: 307-326, 1997) and the statistics from data collection and data refinement are shown in Tables 1 and 2 below, respectively.

Table 1. Statistics for Data Collection and Phase Determination

| Data Collection | mAb13.2 Fab | mAb13.2/IL-13 Fab |
|-------------------------------------|---|------------------------------------|
| Crystal system | Orthorhombic | Cubic |
| Space group | P2 ₁ 2 ₁ 2 ₁ | P2 ₁ 3 |
| Unit cell dimensions | a=54.442, b=97.961, | a=b=c=125.261, |
| | c=108.469, α = β = γ =90.0° | $\alpha=\beta=\gamma=90.0^{\circ}$ |
| Data collection . | -180°C | -180°C |
| temperature | | |
| Number of crystals | 1 | 1 |
| Radiation Source | ALS, Berkeley, CA | ALS, Berkeley, CA |
| Wavelength (Å) | $\lambda = 1.0 \text{ Å}$ | $\lambda = 1.0 \text{ Å}$ |
| Resolution range(Å) | 50-2.8 Å | 50-1.8 Å |
| Maximum resolution (Å) | 2.8 Å | 1.8 Å |
| R _{merge} ^a (%) | 8.2% (38.4%) | 6.7% (48.6%) |
| % complete | 100% (100%) | 99.9% (99.0%) |
| total reflections | 98,254 | 561,539 |
| unique reflections | 14,903 | 57,656 |
| $I/\sigma(I)$ | 23.3 (4.8) | 26.6 (2.8) |

^a $R_{\text{merge}} = \sum |I_h - \langle I_h \rangle| / \sum I_h$, where $\langle I_h \rangle$ is the average intensity over symmetry equivalents. Number in parentheses reflects statistics for the last shell.

Table 2. Structure Refinement Statistics

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| Data Collection | mAb13.2Fab | mAb13.2 Fab/IL-13 |
|---------------------------------|--------------------|---------------------------------|
| Model for molecular replacement | 2E8 Fab (12E8.pdb) | mAb13.2 Fab; soln. |
| | | structure of IL-13 ^b |
| Maximum Resolution (Å) | 2.8 Å | 1.8 Å |
| $R_{work}^{a}(\%)$ | 25.9 % | 20.3 % |
| R _{free} (%) | 30.7 % | 23.5 % |

 $^aR_{work} = \sum ||F_{obs}| - |F_{calc}|| \sum |F_{obs}|$, R_{free} is equivalent to R_{work} , but calculated for a randomly chosen 5% of reflections that are omitted from the refinement process.

^bMoy et al., J. Mol. Biol. <u>310</u>:219-230, 2001.

The structure of mAb13.2 Fab was solved by molecular replacement using the program AMORE (Navaza, *Acta Crystallogr*. <u>A50</u>:157-163, 1994). The structure of the monoclonal 2E8 Fab antibody fragment (PDB code 12E8) was used as the probe. Prior to refinement, 5% of the data were randomly selected and designated as an R_{free} test set to monitor the progress of the refinement. The structure of the mAb13.2 Fab was then rebuilt within QUANTA (Accelrys, San Diego, CA) utilizing a series of omit maps. Following six cycles of refinement with CNS (Brunger *et al.*, *Acta Crystallogr*. <u>D54</u>: 905-921, 1998) and rebuilding using QUANTA, the refinement converged with a model that contained the mAb13.2 Fab and 41 water molecules at

an R_{cryst} of 25.9% and an R_{free} of 30.7%. The structure refinement statistics are shown in Table 2. The crystal structure coordinates are shown in Table 10.

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Example 5. Crystal structure of mAb13.2 Fab/IL-13 Complex. Recombinant IL-13 (Swiss-Prot Accession Number P35225) and mAb13.2 Fab were purified for crystallization. Recombinant IL-13 was purified as follows. *E. coli* K12 strain GI934 was used for expression of Human IL-13. GI934 is an ilvG derivative of GI724 (LaVallie *et al.*, *Bio/Technology* 11:187-193, 1993) that contains specific deletions in the two *E. coli* proteases *omp*T and *omp*P. Specifically, this strain contains the bacteriophage I repressor (cI) gene stably integrated into the chromosomal ampC locus. The cI gene is transcriptionally regulated by a synthetic *Salmonella typhimurium* trp promoter. *E.coli* expression vector pAL-981, a derivative of pAL-781 (Collins-Racie, *et al.*, *Bio/Technology* 13:982-987, 1995), was used as the basis for construction of a Human IL-13 expression vector.

A cDNA of the human IL-13 gene was generated from synthetic oligonucleotide duplexes designed to possess silent changes from human IL-13 cDNA (Accession number NM_002188) that was optimized for E.coli codon usage and increased AT content at the 5' end of the gene. Three sets of complementary duplexes of synthetic oligonucleotides corresponding to amino acids Gly21 to Asn132 of the human IL-13 amino acid (SEQ ID NO:3) (FIG. 2A) were used to construct the mature region of human IL-13, which is the amino acid sequence of processed IL-13 (SEQ ID NO:4). The E. coli optimized complementary oligonucleotides of duplex 1 were 5'-TATGGGTCCAGTTCCACCATCTACTGCTCTGCGTGAACTGATTGAAGAACTGGT TAACATCACCCAGAACCAGAAAGCTCCGCTGTGTAACGGTTCCATGGTTTGGTCCAT CAACCTG-3' (SEQ ID NO:6) with complement 5'-CAGCGGTCAGGTTGATGGACCAAACCATGGAACCGTTACACAGCGGAGCTTTCTG GTTCTGGGTGATGTTAACCAGTTCTTCAATCAGTTCACGCAGAGCAGTAGATGGTGG (SEQ ID NO:7); duplex 2 were AACTGGACCCA-3 5'-ACCGCTGGTATGTACTGTGCAGCTCTGGAATCCCTGATCAACGTTTCTGGTTGC TCTGCTATCGAAAAAACCCAGCGTATGCTGTCTGGTTTCTGCCCGCACAAAGTTTCC GCTGGTCAG-3' (SEQ ID NO:8) with complement 5'-GAGGAGAACTGACCAGCGGAAACTTTGTGCGGGCAGAAACCAGACAGCATACGC TGGGTTTTTTCGATAGCAGAGCAACCAGAAACGTTGATCAGGGATTCCAGAGCTGCA CAGTACATAC-3' (SEQ ID NO:9); and duplex 3 were

5'-TTCTCCTCTGCACGTTCGTGACACCAAAATCGAAGTTGCTCAGTTCGTAAAA GACCTGCTGCACCTGAAAAAACTGTTCCGTGAAGGTCGTTTCAACTAATAAT-

3' (SEQ ID NO:10) with complement

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5'-CTAGATTATTAGTTGAAACGACCTTCACGGAACAGTTTTTTCAGGTGCAGCAGC AGGTCTTTTACGAACTGAGCAACTTCGATTTTGGTGTCACGAACGTGCAGA-3' (SEQ ID NO:11).

The complement (bottom) strand of the first and second duplexes and the top strand of the second and third duplexes were phosphorylated independently. The complementary strands were combined, and each duplex mix was heated to 90°C and then slowly cooled to allow annealing of the duplexes. The first and last duplexes respectively encoded the restriction endonucleases NdeI and XbaI to allow for cloning into an NdeI, XbaI digested and gel purified expression vector pAL-981. All restriction digests, enzymatic phosphorylation of oligonucleotides, DNA fragment isolations and ligations were carried out as described in Sambrook *et al.*, 1989. "Molecular Cloning, a Laboratory Manual, second edition," Cold Spring Harbor Laboratory Press, Cold Spring Harbor, New York. Ligation mixtures were transformed into electrocompetent GI934 as described (LaVallie *et al.*, *Methods Mol Biol.* 205:119-140, 2003). Ligation of the three sets of oligonucleotide duplexes into pAL-981 created plasmid pALHIL13-981. All synthetic oligonucleotides were sequence confirmed after cloning into the expression vector.

The resulting plasmid pALHIL13-981 was transformed into GI934. Optimal growth temperature of the culture for production of human IL-13 from plasmid pALHIL13-981 was determined empirically. Fermentor medium consisted of 1% casamino-acids, 1.75% w/v glucose, 50mM KH₂PO₄, 15mM (NH₄)₂SO₄, 30mM Na₃.citrate.2H₂0, 20mM MgSO₄, 100μg/ml ampicillin, DM trace metals (300μM FeCl₃, 29μM ZnCl₃, 36μM CoCl₂, 25μM Na₂MoO₄, 20μM CaCl₂, 22μM CuCl₂, 24μM H₃BO₃), and was adjusted to pH 7 with NH₄OH. A 10L fermentor was inoculated to A₅₅₀ 0.00005 with a fresh culture of GI934 containing pALHIL13-981 grown in Fermentor medium at 30°C. The fermentor culture was grown at 30°C to A₅₅₀ of 1.2, then the temperature was adjusted to 37°C, and the culture was allowed to grow to A₅₅₀ of 7.5. Induction of protein synthesis from the pL promoter was initiated and the culture with the addition of tryptophan to 500μg/ml. The culture was grown at

37°C for 4.25 hours before harvesting the cells by centrifugation. The sequence of the expression vector is shown in FIG. 13 (SEQ ID NO:5).

The protein was essentially completely insoluble. Cells were broken with a microfluidizer and insoluble IL-13 was collected and dissolved at about 2 mg/mL in 50 mM Ches (pH 9), 6 M Guanidine-HCl, 1 mM EDTA, 20 mM DTT. The solution was diluted 20-fold into 50 mM Ches (pH 9), 3 M guanidine-HCl, 100 mM NaCl, 1 mM oxidized glutathione, and dialyzed twice against ten volumes of 20 mM Mes (pH 6). Following clarification by centrifugation, IL-13 was adsorbed to SP-Sepharose and eluted with a gradient of NaCl in Mes buffer. Final purification was by size-exclusion chromatography in 40 mM sodium phosphate, 40 mM NaCl on Superdex 75.

The mAb13.2 Fab was purified as described in Example 4.

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The Fab:IL-13 complex was prepared by combining the two in a molar ratio of about 1:1. IL-13 (50 μM in 40 mM MES and 40 mM NaCl, pH 6.0) and mAb13.2 Fab (50 μM in 50 mM Tris.HCl, pH 8.0) were mixed together to give a final complex concentration of 50 μM. The complex was further purified by a Superdex 75 size exclusion column (Amersham Biosciences, Piscataway, NJ) equilibrated with 50 mM Tris-HCl and 300 mM NaCl, pH 8.0, at 25°C. The purified complex was dialyzed in 50 mM Tris-HCl and 50 mM NaCl, pH 8.0, before setting up the crystallization.

For crystallization, purified mAb13.2 Fab/II-13 complex was prepared at a concentration of 11.3 mg/mL in a solution of 50 mM Tris (pH 8.0) and 50 mM NaCl. One microliter of protein solution was mixed with 1 µl of crystallization solution (20% PEG 3350, 50 mM ZnOAc) (Hampton Research, Aliso Viejo, CA). The crystals formed at 18°C by vapor diffusion by the hanging drop method.

Data from the crystal of the mAb13.2 Fab/IL-13 complex were collected on beamline 5.0.2 at the ALS (Berkley, CA) using an ADSC Quantum-4 CCD detector. A single crystal, vitrified at -180°C, was used for the data set. The data were processed using DENZO and Scalepack (Otwinowski and Minor, *Methods Enzymol*. 276: 307-326, 1997). The statistics from data refinement are shown in Table 2. The crystal sructure coordinates are shown in Table 11.

Crystals of the binary mAb13.2Fab/IL-13 complex diffracted to 1.8 Å using synchrotron radiation. The structure of the complex was solved by molecular replacement using the program AMORE, and using the crystal structure of the

data were randomly selected and designated as an R_{free} test to monitor the progress of the refinement. This structure of the mAb13.2 Fab was then rebuilt within QUANTA using a series of omit maps. During this process, extra density was observed near the hypervariable regions, and these regions sharpened after each cycle of rebuilding. After the Fab fragment had been rebuilt, the NMR structure of IL-13 (Moy *et al.*, *J. Mol. Biol.* 310:219-230, 2001) was rotated into the density adjacent to the hypervariable regions. Following three cycles of refinement with CNS (Accelrys, San Diego, CA) and rebuilding within QUANTA, the refinement converged with a model that contained one molecule of the mAb13.2 Fab, one molecule of IL-13, one acetate molecule, three zinc ions, and 465 water molecules at an R_{cryst} of 20.3% and R_{free} of 23.5%. The refinement statistics are shown in Table 2.

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In the mAb13.2/IL-13 crystalline complex, residues 1-211 of the Fab light chain were visible, while residues 212, 213, and 214 were not observed in the density. For the heavy chain, residues 1-127 and 133-210 were modeled into the density, and no density was observed for residues 128 to 132. For IL-13, residues 7-21, 26-78, and 81-109 were visible and residues 1-6, 22-25, 79, and 80 were disordered. Several residues modeled as smaller residues due to inadequate electron density X-ray experiments (see Table 5).

There were three zinc molecules from the crystallization buffer that were found bound in this structure. None of them were involved in interactions between the IL-13 and Fab molecules. Two of the zinc molecules were involved in contacts between molecules in the asymmetric unit and symmetry related copies of the proteins, and thus they were important for crystallization of this complex. Zinc1 was coordinated to Fab light chain residues Glu27 and Glu97, and residues Glu189 and His193 of a symmetry related copy of the light chain (amino acids numbered according to SEQ ID NO:1 (FIG. 1A)). Zinc2 was coordinated to IL-13 residues His84 and Asp87, and residues Asp98 and His102 of a symmetry related copy of IL-13. Zinc3 was coordinated to IL-13 residues Glu12 and Glu15 with water molecules as other ligands (amino acids numbered according to SEQ ID NO:4 (FIG. 2B)).

The residues of IL-13 interacting with the mAb13.2 Fab fragment were located at

C alpha helix of IL-13 with the CDR loops of the antibody. Hydrogen bond interactions were observed to exist between the Fab and IL-13 residues Glu49, Asn53, Gly69, Pro72, His73, Lys74, and Arg86. The N-terminal tip of helix A was within van der Waals distances of the Fab fragment. These interactions are summarized in Tables 3 and 4.

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Table 3. H-bond Interactions between IL-13 and Fab 13.2

| | | IL-13 ^a | | | Fab 13.2 | | | |
|----|--------|--------------------|------|---------|----------------------|---------------------|------|----------|
| | Residu | ie | atom | Residue | Chothia ^b | SEQ ID ^c | Atom | Distance |
| 5 | Glu | 49I | OE1 | Asn | 30AL | 31L | ND2 | 2.87Å |
| | Glu | 49I | OE2 | Tyr | 98H | 101H | OH | 2.69 |
| | Glu | 49I | OE2 | Tyr | 99H | 102H | OH | 2.54 |
| | Asn | 53I | OD1 | Lys | 30DL | 34L | NZ | 2.74 |
| | Gly | 69I | 0 | Ser | 53H | 53H | N | 2.91 |
| 10 | Pro | 72I | 0 | Tyr | 98H | 101H | N | 3.10 |
| | His | 73I | ND1 | Asp | 94L | 98L | OD1 | 2.87 |
| | His | 73I | NE2 | Ser | 50H | 50H | OG | 2.75 |
| | Lys | 74I | NZ | Asn | 30AL | 31L | OD1 | 2.95 |
| | Lys | 74I | NZ | Asn | 92L | 96L | OD1 | 2.61 |
| 15 | Arg | 86I | NH1 | Tyr | 30BL | 32L | OH | 3.16 |
| | Arg | 86I | NH2 | Tvr | 30BL | 32L | OH | 2.93 |

^aAmino acid residues are numbered according to the processed form of IL-13 (SEQ ID NO:4). "I" indicates amino acid of IL-13.

^bAmino acid residues correspond to SEQ ID NO:1 (for light chain residues, "L") or SEQ ID NO:2 (for heavy chain residues, "H"), and are numbered according to the Chothia numbering system (Al-Lazikani *et al.*, *Jour. Mol. Biol.* 273:927-948, 1997).

^cAmino acid residues are numbered according to the numbering of SEQ ID NO:1 (for light chain residues, "L") or SEQ ID NO:2 (for heavy chain residues, "H").

Table 4. van der Waals Type Interactions between IL-13 and Fab 13.2

| | IL-13 | | Fab 13 | 3.2 | | | |
|----|--------|-----------------|--------|-----|----------------------|--------|--------|
| | Residu | ıe ^a | Residu | 1e | Chothia ^b | SEQ ID | CDR_ |
| 5 | Ser | 7I | Ile | | 30H | 30H | CDR-H1 |
| | Thr | 8I | Ile | | 30H | 30H | CDR-H1 |
| | Ala | 9I | Ile | | 30H | 30H | CDR-H1 |
| | Ala | 9I | Ser | | 53H | 53H | CDR-H2 |
| | Glu | 12I | Пе | | 30H | 30H | CDR-H1 |
| 10 | Glu | 12I | Ser | | 31H | 31H | CDR-H1 |
| | Leu | 48I | Tyr | | 98H | 101H | CDR-H3 |
| | Glu | 49I | Tyr | | 98H | 101H | CDR-H3 |
| | Glu | 49I | Asn | | 30AL | 31L | CDR-L1 |
| | Glu | 49I | Tyr | | 99H | 102H | CDR-H3 |
| 15 | Ile | 52I | Tyr | | 99H | 102H | CDR-H3 |
| | Ile | 52I | Tyr | | 99H | 102H | CDR-H3 |
| | Ile | 52I | Tyr | | 99H | 102H | CDR-H3 |
| | Ile | 52I | Arg | | 50L | 54L | CDR-L2 |
| | Ile | 52I | Tyr | | 99H | 102H | CDR-H3 |
| 20 | Ile | 52I | Lys | | 30DL | 34L | CDR-L1 |
| | Asn | 53I | Lys | | 30DL | 34L | CDR-L1 |
| | Asn | 53I | Lys | | 30DL | 34L | CDR-L1 |
| | Asn | 53I | Lys | | 30DL | 34L | CDR-L1 |
| | Arg | 65I | Phe | | 100H | 103H | CDR-H3 |
| 25 | Arg | 65I | Asp | | 96H | 99H | CDR-H3 |
| | Met | 66I | Ser | | 31H | 31H | CDR-H1 |
| | Ser | 68I | Asp | | 96H | 99H | CDR-H3 |
| | Ser | 68I | Phe | | 100H | 103H | CDR-H3 |
| | Gly | 69I | Ser | | 31H | 31H | CDR-H1 |
| 30 | Gly | 69I | Ala | | 33H | 33H | CDR-H1 |
| | Gly | 69I | Ser | | 53H | 53H | CDR-H2 |
| | Gly | 69I | Ser | | 52H | 52H | CDR-H2 |
| | Phe | 70 I | Ser | | 53H | 53H | CDR-H2 |
| | Phe | 70I | Ser | | 52H | 52H | CDR-H2 |
| 35 | Cys | 71I | Tyr | | 98H | 101H | CDR-H3 |
| | Pro | 72I | Ala | | 33H | 33H | CDR-H1 |
| | Pro | 72I | Leu | | 95H | 98H | CDR-H3 |
| | Pro | 72I | Ser | | 52H | 52H | CDR-H2 |
| | Pro | 72I | Tyr | | 58H | 58H | CDR-H2 |
| 40 | Pro | 72I | Tyr | | 98H | 101H | CDR-H3 |
| | Pro | 72I | Gly | | 97H | 100H | CDR-H3 |
| | Pro | 72I | Trp | | 96L | 100L | CDR-L3 |
| | His | 73I | Asp | | 94L | 98L | CDR-L3 |
| | His | 73I | Trp | | 96L | 100L | CDR-L3 |
| 45 | His | 73I | Trp | | 47H | 47H | ~~~ |
| | His | 73I | Leu | | 95H | 98H | CDR-H3 |
| | His | 73I | Tyr | 58H | | 58H | CDR-H2 |
| | His | 73I | Ser | 50H | | 50H | CDR-H2 |
| | His | 73I | Tyr | 98H | | 101H | CDR-H3 |

| Lys | 74I | Tyr | 98H | 101H | CDR-H3 |
|-----|-----|-----|------|------|--------|
| Lys | 74I | Asn | 30AL | 31L | CDR-L1 |
| Lys | 74I | Asn | 92L | 96L | CDR-L3 |
| Arg | 86I | Tyr | 30BL | 32L | CDR-L1 |

^aAmino acid residues are numbered according to the processed form of IL-13 (SEQ ID NO:4). "I" indicates amino acid of IL-13.

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Table 5. Residues mis-modeled due to inadequate electron density

| ^c Sequence ^c Mod | eled As |
|--|---|
| Lys Ala | |
| Lys Ala | |
| Gln Ala | |
| Glu Ala | |
| Leu Ala | |
| Lys Ala | |
| Lys Ala | |
| Gln Ala | |
| Lys Ala | |
| • | |
| Lys Ala | |
| • | |
| Arg Ala | |
| | |
| Glu Ala | |
| | Lys Ala Lys Ala Gln Ala Glu Ala Leu Ala Lys Ala Lys Ala Lys Ala Gln Ala Lys Ala Lys Ala Ala Arg Ala |

^a "HC" is heavy chain (SEQ ID NO:2); "LC" is light chain (SEQ ID NO:1); "I" is IL-13 processed (SEQ ID NO:4).

FIG. 3 is a ribbon diagram illustrating the co-crystal structure of mAb13.2 Fab with human IL-13. The light chain of mAb13.2 Fab is shown in dark shading, and the heavy chain in light shading. The IL-13 structure is shown at right. The figure depicts the interaction of the C alpha helix of IL-13 with the CDR loops of the antibody. The major residues of mAb13.2 heavy chain that make hydrogen bond contacts with IL-13 are SER50 (CDR2), SER53 (CDR2), TYR101 (CDR3), and

^bAmino acid residues correspond to SEQ ID NO:1 (for light chain residues, "L") or SEQ ID NO:2 (for heavy chain residues, "H"), and are numbered according to the Chothia numbering system (Al-Lazikani *et al.*, *Jour. Mol. Biol.* 273:927-948, 1997). See Tables 6 and 7.

^cAmino acid residues are numbered according to the numbering of SEQ ID NO:1 (for light chain residues, "L") or SEQ ID NO:2 (for heavy chain residues, "H").

^bAmino acid residues correspond to SEQ ID NO:1 (for light chain residues, "LC") or SEQ ID NO:2 (for heavy chain residues, "HC"), and are numbered according to the Chothia numbering system (Al-Lazikani *et al.*, *Jour. Mol. Biol.* 273:927-948, 1997). See Tables 6 and 7.

^cAmino acid residues are numbered and identified according to the numbering of SEQ ID NO:1 (for light chain residues, "LC"), SEQ ID NO:2 (for heavy chain residues, "HC"), or SEQ ID NO:4 (for residues of the IL-13 processed polypeptide, "I").

TYR102 (CDR3). The major residues of mAb13.2 heavy chain that make van der Waals contacts with IL-13 are ILE30 (CDR1), SER31 (CDR1), ALA33 (CDR1), TRP47, SER50 (CDR2), SER52 (CDR2), SER53 (CDR2), TYR58 (CDR2), LEU98 (CDR3), ASP99 (CDR3), GLY100 (CDR3), TYR101 (CDR3), TYR102 (CDR3), and PHE103 (CDR3) (see Table 4; amino acids numbered according the numbering of SEQ ID NO:2 (FIG. 1B)).

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According to the amino acid numbering of SEQ ID NO:1 (FIG. 1A), the major residues of mAb13.2 light chain that make hydrogen bond contacts with IL-13 are ASN31 (CDR1), TYR32 (CDR1), LYS34 (CDR1), ASN96 (CDR3), and ASP98 (CDR3). The major residues of mAb13.2 light chain that make van der Waals contacts with IL-13 are ASN31 (CDR1), TYR32 (CDR1), LYS34 (CDR1), ARG54 (CDR2), ASN96 (CDR3), ASP98 (CDR3), and TRP100 (CDR3) (see Table 4).

Various numbering schemes have evolved to describe the amino acid residues of the heavy and light chain polypeptides of an antibody. The Kabat and Chothia schemes number the amino acid residues linearly accept in the defined CDR region of the polypeptide, where insertions are noted. The Kabat system (Kabat *et al.*, NIH Publ. No. 91-3242, 5th ed., vols. 1-3, Dept. of Health and Human Services, 1991) defines the location of the heavy and light chain CDRs by sequence variability, while the Chothia system (Al-Lazikani *et al.*, *Jour. Mol. Biol.* 273:927-948, 1997) defines the location structurally by loop regions. Because of the different placement of the CDR insertions, the numbering of the amino acids in the heavy chain and light chain can vary between the two systems. The notation of amino acid insertions causes each of these numbering systems to deviate from the linear numbering. Tables 6 and 7 align the amino acid sequences of the light and heavy chains, respectively, of mAb13.2Fab according to these three different numbering schemes (Kabat, Chothia, and linear numbering).

Table 6. Amino acid sequence of the light chain of mAb13.2Fab according to the linear (SEQ ID NO:1), Chothia and Kabat numbering systems.^a

| Residue | Linear Sequence Number | Chothia Structure Number | Kabat Sequence Number |
|---------|------------------------------|--------------------------------|-----------------------------|
| D | 1 | 1 | 1 |
| I | 2 | 2 | 2 |
| V | 3 | 3 | 3 |
| L | 4 | 4 | 4 |
| ${f T}$ | 5 | 5 | 5 |
| Q | 6 | 6 | 6 |
| S | 7 | 7 | 7 |
| P | 8 | 8 | 8 |
| A | 9 | 9 | 9 |
| S | 10 | 10 | 10 |
| L | 11 | 11 | 11 |
| A | 12 | 12 | 12 |
| V | 13 | 13 | 13 |
| S | 14 | 14 | 14 |
| L | 15 | 15 | 15 |
| G | 16 | 16 | 16 |
| Q | 17 | 17 | 17 |
| R | 18 | 18 | 18 |
| A | 19 | 19 | 19 |
| ${f T}$ | 20 | 20 | 20 |
| I | 21 | 21 | 21 |
| s | 22 | · 22 | 22 |
| C | 23 | 23 | 23 |
| K | 24 | 24 | 24 |
| A | 25 | 25 | 25 |
| S | 26 | 26 | 26 |
| E | 27 | 27 | 27 |
| S | 28 | 28 | 27A |
| V | 29 | 29 | 27B |
| D | 30 | 30 | 27C |
| N | 31 | 30A | 27D |
| Y | 32 | 30B | 28 |
| G | 33 | 30C | 29 |
| K | 34 | 30D | 30 |
| S | 35 | 31 | 31 |
| L | 36 | 32 | 32 |

| M | 37 | 33 | 33 |
|--------------|--------|----------|----------|
| H | 38 | 34 | 34 |
| W | 39 | 35 | 35 |
| Y | 40 | 36 | 36 |
| Q | 41 | 37 | 37 |
| Q | 42 | 38 | 38 |
| K | 43 | 39 | 39 |
| P | 44 | 40 | 40 |
| G | 45 | 41 | 41 |
| Q | 46 | 42 | 42 |
| S | 47 | 43 | 43 |
| P | 48 | 44 | 44 |
| K | 49 | 45 | 45 |
| L | 50 | 46 | 46 |
| L | 51 | 47 | 47 |
| I | 52 | 48 | 48 |
| Y | 53 | 49 | 49 |
| R | 54 | 50 | 50 |
| A | 55 | 51 | 51 |
| S | 56 | 52 | 52 |
| N | 57 | 53 | 53 |
| L | 58 | 54 | 54 |
| E | 59 | 55 | 55 |
| S | 60 | 56 | 56 |
| G | 61 | 57 | 57 |
| I | 62 | 58 | 58 |
| P | 63 | 59 | 59 |
| A | 64 | 60 | 60 |
| R | 65 | 61 | 61 |
| F | 66 | 62 | 62 |
| S | 67 | 63 | 63 |
| G | 68 | 64 | 64 |
| S | 69 | 65 | 65 |
| G | 70 | 66 | 66 |
| S | 71 | 67 | 67 |
| R | 72 | 68 | 68 |
| ${f T}$ | 73 | 69 | 69 |
| D | 74 | 70 | 70 |
| F | 75 | 71 | 71 |
| ${f T}$ | 76 | 72 70 | 72 73 |
| L | 77 | 73 74 | 73 74 |
| \mathbf{T} | 78 | 74 75 | 74 75 |
| I | 79 | 75 70 | 75 76 |
| N | 80 | 76 | 76 50 |
| | | | 20 |

| P | 81 | 77 | 77 |
|----------|------------|------------|------------|
| V | 82 | 78 | 78 |
| E | 83 | 79 | 79 |
| A | 84 | 80 | 80 |
| D | 85 | 81 | 81 |
| D | 86 | 82 | 82 |
| V | 87 | 83 | . 83 |
| A | 88 | 84 | 84 |
| ${f T}$ | 89 | 85 | 85 |
| Y | 90 | 86 | 86 |
| Y | 91 | 87 | 87 |
| C | 92 | 88 | 88 |
| Q | 93 | 89 | 89 |
| Q | 94 | 90 | 90 |
| S | 95 | 91 | 91 |
| N | 96 | 92 | 92 |
| E | 97 | 93 | 93 |
| D | 98 | 94 | 94 |
| P | 99 | 95 | 95 |
| M | 100 | 96 | 96 |
| ${f T}$ | 101 | 97 | 97 |
| F | 102 | 98 | 98 |
| G | 103 | 99 | 99 |
| G | 104 | 100 | 100 |
| G | 105 | 101 | 101 |
| T | 106 | 102 | 102 |
| K | 107 | 103 | 103 |
| L | 108 | 104 | 104 |
| E | 109 | 105 | 105 |
| I | 110 | 106 | 106 |
| K | 111 | 107 | 107 |
| <u>R</u> | <u>112</u> | <u>108</u> | <u>108</u> |
| A | 113 | 109 | 109 |
| D | 114 | 110 | 110 |
| A | 115 | 111 | 111 |
| A | 116 | 112 | 112 |
| P | 117 | 113 | 113 |
| ${f T}$ | 118 | 114 | 114 |
| V | 119 | 115 | 115 |
| S | 120 | 116 | 116 |
| I | 121 | 117 | 117 |
| F | 122 | 118 | 118 |
| P | 123 | 119 | 119 |
| P | 124 | 120 | 120 |
| | | | <i>E</i> 1 |

| | S | 125 | 121 | 121 |
|---|---|-----|-----|-----|
| | S | 126 | 122 | 122 |
| | E | 127 | 123 | 123 |
| | Q | 128 | 124 | 124 |
| | L | 129 | 125 | 125 |
| | T | 130 | 126 | 126 |
| | S | 131 | 127 | 127 |
| | G | 132 | 128 | 128 |
| | G | 133 | 129 | 129 |
| | A | 134 | 130 | 130 |
| | S | 135 | 131 | 131 |
| | V | 136 | 132 | 132 |
| | V | 137 | 133 | 133 |
| | C | 138 | 134 | 134 |
| | F | 139 | 135 | 135 |
| | L | 140 | 136 | 136 |
| | N | 141 | 137 | 137 |
| | N | 142 | 138 | 138 |
| | F | 143 | 139 | 139 |
| | Y | 144 | 140 | 140 |
| | P | 145 | 141 | 141 |
| | K | 146 | 142 | 142 |
| | D | 147 | 143 | 143 |
| | I | 148 | 144 | 144 |
| | N | 149 | 145 | 145 |
| | V | 150 | 146 | 146 |
| | K | 151 | 147 | 147 |
| | M | 152 | 148 | 148 |
| | K | 153 | 149 | 149 |
| | I | 154 | 150 | 150 |
| | D | 155 | 151 | 151 |
| | G | 156 | 152 | 152 |
| | S | 157 | 153 | 153 |
| | E | 158 | 154 | 154 |
| | R | 159 | 155 | 155 |
| | Q | 160 | 156 | 156 |
| | N | 161 | 157 | 157 |
| | G | 162 | 158 | 158 |
| | V | 163 | 159 | 159 |
| | L | 164 | 160 | 160 |
| | N | 165 | 161 | 161 |
| | S | 166 | 162 | 162 |
| | W | 167 | 163 | 163 |
| 1 | T | 168 | 164 | 164 |

| D | 169 | 165 | 165 |
|--------------|-----|-------|-----|
| Q | 170 | 166 | 166 |
| D | 171 | 167 | 167 |
| S | 172 | 168 | 168 |
| K | 173 | 169 | 169 |
| D | 174 | 170 | 170 |
| S | 175 | 171 | 171 |
| ${f T}$ | 176 | 172 | 172 |
| Y | 177 | 173 | 173 |
| S | 178 | 174 | 174 |
| M | 179 | 175 | 175 |
| S | 180 | 176 · | 176 |
| S | 181 | 177 | 177 |
| ${f T}$ | 182 | 178 | 178 |
| L | 183 | 179 | 179 |
| ${f T}$ | 184 | 180 | 180 |
| L | 185 | 181 | 181 |
| ${f T}$ | 186 | 182 | 182 |
| K | 187 | 183 | 183 |
| D | 188 | 184 | 184 |
| E | 189 | 185 | 185 |
| Y | 190 | 186 | 186 |
| E | 191 | 187 | 187 |
| R | 192 | 188 | 188 |
| H | 193 | 189 | 189 |
| N | 194 | 190 | 190 |
| S | 195 | 191 | 191 |
| Y | 196 | 192 | 192 |
| ${f T}$ | 197 | 193 | 193 |
| C | 198 | 194 | 194 |
| E | 199 | 195 | 195 |
| A | 200 | 196 | 196 |
| ${f T}$ | 201 | 197 | 197 |
| H | 202 | 198 | 198 |
| K | 203 | 199 | 199 |
| ${f T}$ | 204 | 200 | 200 |
| S | 205 | 201 | 201 |
| \mathbf{T} | 206 | 202 | 202 |
| S | 207 | 203 | 203 |
| P | 208 | 204 | 204 |
| I | 209 | 205 | 205 |
| V | 210 | 206 | 206 |
| K | 211 | 207 | 207 |
| S | 212 | 208 | 208 |
| | | | 53 |

| F | 213 | 209 | 209 |
|---|-----|-----|-----|
| N | 214 | 210 | 210 |
| R | 215 | 211 | 211 |
| N | 216 | 212 | 212 |
| E | 217 | 213 | 213 |
| C | 218 | 214 | 214 |

^aBold font indicates an insertion in the linear sequence according to the Chothia or Kabat numbering system. Bold and underlined residue indicates an insertion as determined by X-ray data.

Table 7. Amino acid sequence of the heavy chain of mAb13.2Fab according to the linear (SEQ ID NO:2), Chothia and Kabat numbering systems.^a

| Residue | <u>Linear</u> <u>Sequence</u> <u>Number</u> | Chothia Structure Number | <u>Kabat</u> <u>Sequence</u> <u>Number</u> |
|---------|---|--------------------------------|--|
| E | 1 | 1 | 1 |
| V | 2 | 2 | 2 |
| K | 3 | 3 | 3 |
| L | 4 | 4 | 4 |
| V | 5 | 5 | 5 |
| E | 6 | 6 | 6 |
| S | 7 | 7 | 7 |
| G | 8 | 8 | 8 |
| G | 9 | 9 | 9 |
| G | 10 | 10 | 10 |
| L | 11 | 11 | 11 |
| V | 12 | 12 | 12 |
| K | 13 | 13 | 13 |
| P | 14 | 14 | 14 |
| G | 15 | 15 | 15 |
| G | 16 | 16 | 16 |
| S | 17 | 17 | 17 |
| L | 18 | 18 | 18 |
| K | 19 | 19 | 19 |
| L | 20 | 20 | 20 |
| S | 21 | 21 | 21 |
| C | 22 | 22 | 22 |
| A | 23 | 23 | 23 |
| A | 24 | 24 | 24 |
| S | 25 | 25 | 25 |
| G | 26 | 26 | 26 |
| F | 27 | 27 | 27 |
| T | 28 | 28 | 28 |
| F I | 29 30 | 29 30 | 29 30 |
| S | 31 | 31 | 31 |
| Y | 32 | 32 | 32 |
| A | 33 | 33 | 33 |
| M | 34 | 34 | 34 |
| S | 35 | 35 | 35 |

| W | 36 | 36 | 36 |
|---------|----|----|----|
| V | 37 | 37 | 37 |
| R | 38 | 38 | 38 |
| Q | 39 | 39 | 39 |
| T | 40 | 40 | 40 |
| P | 41 | 41 | 41 |
| E | 42 | 42 | 42 |
| K | 43 | 43 | 43 |
| R | 44 | 44 | 44 |
| L | 45 | 45 | 45 |
| E | 46 | 46 | 46 |
| M | 47 | 47 | 47 |
| V | 48 | 48 | 48 |
| A | 49 | 49 | 49 |
| S | 50 | 50 | 50 |
| I | 51 | 51 | 51 |
| S | 52 | 52 | 52 |
| S | 53 | 53 | 53 |
| G | 54 | 54 | 54 |
| G | 55 | 55 | 55 |
| N | 56 | 56 | 56 |
| T | 57 | 57 | 57 |
| Y | 58 | 58 | 58 |
| Y | 59 | 59 | 59 |
| P | 60 | 60 | 60 |
| D | 61 | 61 | 61 |
| s | 62 | 62 | 62 |
| V | 63 | 63 | 63 |
| K | 64 | 64 | 64 |
| G | 65 | 65 | 65 |
| R | 66 | 66 | 66 |
| F | 67 | 67 | 67 |
| ${f T}$ | 68 | 68 | 68 |
| I | 69 | 69 | 69 |
| S | 70 | 70 | 70 |
| R | 71 | 71 | 71 |
| D | 72 | 72 | 72 |

| N | 73 | 73 | 73 |
|---|-----|------|------|
| A | 74 | 74 | 74 |
| R | 75 | 75 | 75 |
| N | 76 | 76 | 76 |
| I | 77 | 77 | 77 |
| L | 78 | 78 | 78 |
| Y | 79 | 79 | 79 |
| L | 80 | 80 | 80 |
| Q | 81 | 81 | 81 |
| M | 82 | 82 | 82 |
| s | 83 | 82A | 82A |
| s | 84 | 82B | 82B |
| L | 85 | 82C | 82C |
| R | 86 | 83 | 83 |
| S | 87 | 84 | 84 |
| E | 88 | 85 | 85 |
| D | 89 | 86 | 86 |
| T | 90 | 87 | 87 |
| A | 91 | 88 | 88 |
| M | 92 | 89 | 89 |
| Y | 93 | 90 | 90 |
| Y | 94 | 91 | 91 |
| C | 95 | 92 | 92 |
| A | 96 | 93 | 93 |
| R | 97 | 94 | 94 |
| L | 98 | 95 | 95 |
| D | 99 | 96 | 96 |
| G | 100 | 97 | 97 |
| Y | 101 | 98 | 98 |
| Y | 102 | 99 | 99 |
| F | 103 | 100 | 100 |
| G | 104 | 100A | 100A |
| F | 105 | 100B | 100B |
| A | 106 | 101 | 101 |
| Y | 107 | 102 | 102 |
| W | 108 | 103 | 103 |
| G | 109 | 104 | 104 |

| Q | 110 | 105 | 105 |
|----------|------------|------------|------------|
| G | 111 | 106 | 106 |
| T | 112 | 107 | 107 |
| L | 113 | 108 | 108 |
| V | 114 | 109 | 109 |
| A | 115 | 110 | 110 |
| V | 116 | 111 | 111 |
| S | 117 | 112 | 112 |
| A | 118 | 113 | 113 |
| A | 119 | 114 | 114 |
| <u>K</u> | <u>120</u> | <u>115</u> | <u>115</u> |
| T | 121 | 116 | 116 |
| ${f T}$ | 122 | 117 | 117 |
| P | 123 | 118 | 118 |
| P | 124 | 119 | 119 |
| S | 125 | 120 | 120 |
| V | 126 | 121 | 121 |
| Y | 127 | 122 | 122 |
| P | 128 | 123 | 123 |
| Ŀ | 129 | 124 | 124 |
| A | 130 | 125 | 125 |
| P | 131 | 126 | 126 |
| G | 132 | 127 | 127 |
| S | 133 | 128 | 128 |
| A | . 134 | 129 | 129 |
| A | 135 | 130 | 130 |
| Q | 136 | 131 | 131 |
| ${f T}$ | 137 | 132 | 132 |
| N | 138 | 133 | 133 |
| s | 139 | 134 | 134 |
| M | 140 | 135 | 135 |
| V | 141 | 136 | 136 |
| ${f T}$ | 142 | 137 | 137 |
| L | 143 | 138 | 138 |
| G | 144 | 139 | 139 |
| С | 145 | 140 | 140 |
| L | 146 | 141 | 141 |

| V | 147 | 142 | 142 |
|---------|-----|-----|-----|
| K | 148 | 143 | 143 |
| G | 149 | 144 | 144 |
| Y | 150 | 145 | 145 |
| F | 151 | 146 | 146 |
| P | 152 | 147 | 147 |
| E | 153 | 148 | 148 |
| P | 154 | 149 | 149 |
| Λ | 155 | 150 | 150 |
| ${f T}$ | 156 | 151 | 151 |
| V | 157 | 152 | 152 |
| ${f T}$ | 158 | 153 | 153 |
| W | 159 | 154 | 154 |
| N | 160 | 155 | 155 |
| S | 161 | 156 | 156 |
| G | 162 | 157 | 157 |
| S | 163 | 158 | 158 |
| L | 164 | 159 | 159 |
| S | 165 | 160 | 160 |
| S | 166 | 161 | 161 |
| G . | 167 | 162 | 162 |
| V | 168 | 163 | 163 |
| H | 169 | 164 | 164 |
| T | 170 | 165 | 165 |
| F | 171 | 166 | 166 |
| P | 172 | 167 | 167 |
| A | 173 | 168 | 168 |
| V | 174 | 169 | 169 |
| L | 175 | 170 | 170 |
| E | 176 | 171 | 171 |
| S | 177 | 172 | 172 |
| D | 178 | 173 | 173 |
| L | 179 | 174 | 174 |
| Y | 180 | 175 | 175 |
| ${f T}$ | 181 | 176 | 176 |
| L | 182 | 177 | 177 |
| S | 183 | 178 | 178 |

| 184 | 179 | 179 |
|-----|---|---|
| 185 | 180 | 180 |
| 186 | 181 | 181 |
| 187 | 182 | 182 |
| 188 | 183 | 183 |
| 189 | 184 | 184 |
| 190 | 185 | 185 |
| 191 | 186 | 186 |
| 192 | 187 | 187 |
| 193 | 188 | 188 |
| 194 | 189 | 189 |
| 195 | 190 | 190 |
| 196 | 191 | 191 |
| 197 | 192 | 192 |
| 198 | 193 | 193 |
| 199 | 194 | 194 |
| 200 | 195 | 195 |
| 201 | 196 | 196 |
| 202 | 197 | 197 |
| 203 | 198 | 198 |
| 204 | 199 | 199 |
| 205 | 200 | 200 |
| 206 | 201 | 201 |
| 207 | 202 | 202 |
| 208 | 203 | 203 |
| 209 | 204 | 204 |
| 210 | 205 | 205 |
| 211 | 206 | 206 |
| 212 | 207 | 207 |
| 213 | 208 | 208 |
| 214 | 209 | 209 |
| 215 | 210 | 210 |
| | 185 186 187 188 189 190 191 192 193 194 195 196 197 198 199 200 201 202 203 204 205 206 207 208 209 210 211 212 213 214 | 185 180 186 181 187 182 188 183 189 184 190 185 191 186 192 187 193 188 194 189 195 190 196 191 197 192 198 193 199 194 200 195 201 196 202 197 203 198 204 199 205 200 206 201 207 202 208 203 209 204 210 205 211 206 212 207 213 208 214 209 |

^aBold font indicates an insertion in the linear sequence according to the Chothia or Kabat numbering system. Bold and underlined residue indicates an insertion as determined by X-ray data.

Example 6. Crystal Structure of the Trimeric Complex of Interleukin-13, Il-13 receptor α1, and the Binding Domain of the Inhibitory antibody mAb13.2 Fab.

The extracellular domain (residues 27-342; see FIG. 14) of IL-13Ra1 was expressed with a 6xHis tag fused at the C-terminus (Aman *et al., J. Biol. Chem.* 271:29265-29270, 1996). Expression was performed in the yeast *Pichia pastoris*. The recombinant protein was purified to homogeneity by affinity chromatography over NiNTA-agarose (Qiagen) followed by anion exchange chromatography over HiTrap Q Sepharose HP (Pharmacia, Amersham Pharmacia Biotech, UK) and gel filtration chromatography over Superdex-75 (Pharmacia).

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The human IL-13 (amino acid residues 1 to 113) (SEQ ID NO:4) was expressed and purified as described in example 5.

A complex containing IL-13 and IL-13Rα1 was was formed by mixing the receptor with a slight excess of IL-13. Following confirmation of complex formation by analytical size-exclusion chromatography, the complex was treated with endoglycosidase Hf (endoHf) (25,000 units/mL) for 90 minutes at 37°C. The deglycosylated complexes were applied to a concanavalin A (conA)-Sepharose column to remove protein with uncleaved oligosaccharides, and the remaining complexes were applied to a NiNTA column to remove EndoHf. The purified complexes were purified to homogeneity by gel filtration chromatography over Superdex-200 (GE Healthcare, formerly Amersham Biosciences, Piscatway, NJ). Formation of 1:1 complexes of IL-13 and IL-13Rα1 was confirmed by native polyacrylamide gel electrophoresis and size exclusion chromatography prior to crystal screening.

mAb13.2 Fab was purified as described in example 4.

Crystals of a complex of IL-13, IL-13R α 1, and mAb13.2 Fab were grown at 18°C by vapor diffusion in hanging drops containing 10 mg/ml protein complex, 13% PEG-MME 2000 and 100 mM HEPES (pH 7.0). Crystals appeared in several weeks, but did not reach maximal size for several months. The crystals had the symmetry of space group I4 with unit cell dimensions a = 164.9 Å, b = 164.9 Å, and c = 74.8 Å. Prior to data collection, crystals were briefly transferred to 10% ethylene glycol plus mother liquor and flash cooled in liquid nitrogen. Throughout data collection, the crystal was maintained at 100K. Data were collected at the 5.0.1 beam line at the Advanced Light Source, Berkeley, California. Intensities were integrated and scaled

using DENZO (Otwinowski and Minor, Methods Enzymol. 276:307-326, 1997) and SCALA ("CCP4," Acta Cryst <u>D50</u>:760-763, 1994).

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The structure was solved by molecular replacement using the coordinates of the mAb13.2 Fab/IL-13 complex (Table 11). Initial phases were improved by solvent flattening using Solomon as implemented in CCP4 ("CCP4," Acta Cryst D50:760-763, 1994). Rigid body refinement within CCP4 was used to obtain an initial model. Experimental maps with continuous density were obtained, and an initial model was constructed using QUANTA (Accelrys, Inc., San Diego, CA) and refined against data from 30 to 2.2 Å with CNS (Brunger et al., Acta Cryst. D54:905-921, 1998). The final refined model, which includes polypeptide chains of IL-13Ra1 (residues 6-314), mAb13.2 Fab (light chain residues 1-213 and heavy chain residues 1-213) and IL-13 (residues 6-112), as well as 123 water molecules, has a working R-value of 24.4% and a free R-value of 27.2%. Statistics for data collection and refinement are shown in Tables 8 and 9. There were no backbone torsion angles outside of the allowed regions of the Ramachandran plot. Structural figures were generated using PYMOL (DeLano, "The PYMOL Molecular Graphics System" (2002) DeLano Scientific, San Carlos, CA) and Ribbons (Carson, J.Appl.Cryst. 24:958-961, 1991). The structural coordinates are provided in Table 12. The following residues of IL-13Ra1 had no density beyond the C-beta atom and the coordinates for each were truncated to reflect that ambiguity: 81E, 93R, 104T, 105N, 111S, 112I, 122E, 124D, 150R, 151T, 157N, 165R, 168E, 169K, 174E, 195S, 196S, 197F, 305D, 306T, 339K, 110P, 200Q, 203Q, 204I, 209N, 212K, 213I, 214K, 240N, 279E, 284N, and 293N.

Table 8. Statistics for Data Collection and Phase Determination

| Data Collection | IL-13/mAb13.2 Fab/IL-13Rα1 |
|-------------------------------------|------------------------------------|
| Crystal system | Tetragonal |
| Space group | I 4 |
| Unit cell dimensions | a=b=164.9 Å, c = 74.8 Å, |
| | $\alpha=\beta=\gamma=90.0^{\circ}$ |
| Data collection temperature | 100K |
| Number of crystals | 1 |
| Radiation Source | ALS, Berkeley, CA |
| Wavelength (Å) | $\lambda = 1.0 \text{ Å}$ |
| Resolution range(Å) | 30-2.2 Å |
| Maximum resolution (Å) | 2.2 Å |
| R _{merge} ^a (%) | 6.7% (48.6%) |
| % complete | 99.9% (99.0%) |
| total reflections (free) | 42298 (2110) |
| unique reflections | 40188 |
| I/σ(I) | 26.6 (2.8) |

^a $R_{\text{merge}} = \sum |I_h - \langle I_h \rangle| / \sum I_h$, where $\langle I_h \rangle$ is the average intensity over symmetry equivalents. Number in parentheses reflects statistics for the last resolution shell (2.8 Å -2.7 Å).

Table 9. Structure Refinement Statistics

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| Data Collection | IL-13/mAb13.2 Fab/IL-13Rα1 |
|------------------------------------|----------------------------|
| Model for molecular replacement | mAb13.2 Fab/IL-13 |
| Maximum Resolution (Å) | 2.2 Å |
| R _{work} ^a (%) | 24.4 % |
| R _{free} (%) | 27.2 % |

 $[^]aR_{work} = \sum ||F_{obs}| - |F_{calc}||/\sum |F_{obs}|$, R_{free} is equivalent to R_{work} , but calculated for a randomly chosen 6.4% of reflections that are omitted from the refinement process.

There are two points of substantial interaction between IL-13 and IL-13Rα1. One interaction is between Ig domain 1 and a portion of the loop connecting helices C and D of the cytokine while the other interaction is between Ig domain 3 of the receptor and helices A and D of IL-13 (see FIG. 15).

The interaction between Ig domain 1 of IL-13Ra1 and IL-13 results in the formation of an extended beta sheet spanning the two molecules. Residues Thr88, Lys89, Ile90 and Glu91 of IL-13 (SEQ ID NO:4) form a beta strand that interacts with residues Lys76, Lys77, Ile78 and Ala79 of the receptor (SEQ ID NO:12) (See FIG. 16). Additionally, the side chain of Met33 of IL-13 extends into a hydrophobic pocket that is created by the side chains of these adjoining strands.

The predominant feature of the interaction with Ig domain 3 is the insertion of a hydrophobic residue (Phe107) of IL-13 into a hydrophobic pocket in Ig domain 3 of

the receptor IL-13R α 1. The hydrophobic pocket of IL-13R α 1 is formed by the side chains of residues Leu319, Cys257, Arg256 and Cys320 (FIG. 17). The interaction with Phe107 of IL-13 results in an extensive set of Van der Waals interactions between amino acid residues Ile254, Ser255, Arg256, Lys318, Cys320, and Tyr321 of IL-13R α 1 (SEQ ID NO:12) and amino acid residues Arg11, Glu12, Leu13, Ile14, Glu15, Lys104, Lys105, Leu106, Phe107 and Arg108 of IL-13 (SEQ ID NO:4) (See FIG. 17).

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| | | <u>Table</u> | 10. | Struc | cture | coor | dinates | of mAb13 | 3.2 Fabª | ь | | | |
|----|--------------|----------------|-----------|----------------|--------|------|------------------|------------------|-----------------|----------------|----------------|------------|--------|
| | | # | Name | Res. | Chain | Res | # x | Y | Z | occ | В | SegI | D Ele |
| 5 | ATOM ATOM | 1 2 | N CA | ASP I | | | 5.849 5.758 | -2.062 -0.620 | 0.182 0.381 | | 66.67 65.86 | Ŀ | N |
| • | ATOM | 3 | C | ASP I | | | 7.071 | 0.081 | 0.023 | | 58.91 | r F | C |
| | ATOM | 4 | Ö | ASP I | | | 8.115 | -0.534 | -0.151 | | 57.75 | r. | o |
| | ATOM | 5 | CB | ASP I | | | 5.413 | -0.362 | 1.849 | | 70.47 | L | č |
| 40 | ATOM | 6 | CG | ASP I | | | 6.620 | -0.695 | 2.715 | 1.00 | 75.61 | L | Ċ |
| 10 | MOTA | 7 | | ASP I | | | 7.623 | -1.136 | 2.154 | | 80.71 | L | 0 |
| | ATOM ATOM | 8 9 | | ASP I | | | 6.547 | -0.509 | 3.927 | | 87.49 | L | 0 |
| | ATOM | 10 | N CA | ILE I | | | 6.981 8.171 | $1.415 \\ 2.181$ | -0.125 | | 52.10 | L | N |
| | ATOM | 11 | C | ILE I | | | 8.900 | 2.695 | -0.476 0.767 | | 40.08 42.02 | L L | C C |
| 15 | ATOM | 12 | Õ | ILE I | | | 8.355 | 3.411 | 1.598 | | 48.63 | L | Ö |
| | ATOM | 13 | CB | ILE I | 2 | | 7.740 | 3.360 | -1.351 | | 42.36 | L | č |
| | ATOM | 14 | | ILE I | | | 7.395 | 2.872 | -2.761 | | 38.52 | L | č |
| | MOTA | 15 | | ILE I | | | 8.895 | 4.371 | -1.472 | | 36.85 | L | C |
| 20 | ATOM ATOM | 16 17 | N | ILE I VAL I | | | 7.183 | 4.027 | -3.741 | | 31.90 | L | C |
| 20 | ATOM | 18 | CA | VAL I | | | 10.170 10.965 | 2.268 2.713 | 0.899 2.037 | | 43.87 41.50 | ŗ | N |
| | ATOM | 19 | C | VAL I | | | 11.652 | 4.052 | 1.752 | | 39.10 | L L | C |
| | ATOM | 20 | Ō | VAL I | | | 12.512 | 4.166 | 0.888 | | 45.89 | L | C O |
| | MOTA | 21 | CB | VAL I | | | 12.016 | 1.642 | 2.333 | | 42.05 | L | Č |
| 25 | ATOM | 22 | | VAL I | | | 12.810 | 2.022 | 3.582 | 1.00 | | L | C |
| | ATOM ATOM | 23 24 | | VAL I | | | 11.342 | 0.302 | 2.559 | | 39.67 | L | C |
| | ATOM | 25 | N CA | LEU I | | | 11.341 12.027 | 4.998 6.277 | 2.628 | | 40.82 | Ţ | N |
| | ATOM | 26 | C | LEU I | | | 12.991 | 6.250 | 2.650 3.819 | | 39.96 40.04 | L L | C |
| 30 | ATOM | 27 | ō | LEU I | | | 12.615 | 5.894 | 4.936 | | 41.74 | r r | C O |
| | ATOM | 28 | CB | LEU I | 4 | | 11.036 | 7.412 | 2.857 | | 38.52 | L | č |
| | ATOM | 29 | CG | LEU I | | | 9.763 | 7.348 | 2.031 | | 38.66 | L | Č |
| | ATOM | 30 | | LEU I | | | 9.007 | 8.640 | 2.245 | | 50.64 | L | С |
| 35 | ATOM ATOM | 31 32 | N CD2 | LEU I | | | 10.094 14.234 | 7.164 | 0.562 | | | Ŀ | C |
| 00 | MOTA | 33 | CA | THR I | | | 15.233 | 6.630 6.639 | 3.567 4.622 | | 38.94 41.89 | Ļ | N |
| | ATOM | 34 | C | THR L | | | 15.751 | 8.050 | 4.829 | | 46.14 | L L | C |
| | ATOM | 35 | 0 | THR L | | | 16.433 | 8.595 | 3.962 | | 53.43 | L | ŏ |
| 40 | ATOM | 36 | CB | THR L | | | 16.397 | 5.730 | 4.243 | | 39.78 | L | С |
| 40 | ATOM ATOM | 37 38 | | THR L | | | 15.896 | 4.411 | 3.995 | | 53.91 | L | 0 |
| | ATOM | 39 | N CGZ | GLN L | | | 17.430 15.429 | 5.688 8.664 | 5.347 5.959 | | 41.58 43.43 | Ļ | C |
| | MOTA | 40 | ĈA | GLN L | | | 15.925 | 10.015 | 6.179 | | 44.62 | L L | N C |
| | MOTA | 41 | C | GLN L | | | 17.355 | 9.954 | 6.681 | | 46.70 | L | Č |
| 45 | ATOM | 42 | 0 | GLN L | | | 17.758 | 8.989 | 7.326 | | 45.08 | . L | ŏ |
| | ATOM | 43 | CB | GLN L | | | 15.052 | 10.780 | 7.179 | | 44.41 | L | C |
| | ATOM ATOM | 44 45 | CG | GLN L | | | 13.596 | 10.849 | 6.764 | | 37.31 | Ţ | C |
| | ATOM | 46 | CD OE1 | GLN L | | | 12.796 11.606 | 11.858 11.679 | 7.553 7.762 | | 27.04 | Ŀ | C |
| 50 | MOTA | $\frac{1}{47}$ | | GLN L | | | 13.441 | 12.929 | 7.979 | | 41.69 38.94 | L L | N O |
| | ATOM | 48 | N | SER L | | | 18.117 | 10.993 | 6.364 | | 49.55 | L | N |
| | ATOM | 49 | CA | SER L | | | 19.511 | 11.091 | 6.763 | | 49.16 | L | ĉ |
| | ATOM | 50 | C | SER L | | | 19.823 | 12.568 | 6.912 | | 44.38 | L | C |
| 55 | MOTA MOTA | 51 52 | O | SER L | 7 | | 19.517 | 13.358 | 6.033 | | 48.04 | Ļ | 0 |
| 00 | ATOM | 53 | CB OG | SER L | 7 7 | | 20.399 21.712 | 10.483 10.254 | 5.676 6.152 | | 51.89 68.31 | L | C |
| | ATOM | 54 | N | PRO L | | | 20.426 | 12.960 | 8.037 | | 44.47 | L L | O |
| | MOTA | 55 | | PRO L | 8 | | 20.799 | 12.057 | 9.120 | | 47.06 | Ŀ | C N |
| | MOTA | 56 | C | PRO L | 8 | | 19.607 | 11.777 | 10.028 | | 50.00 | L | č |
| 60 | ATOM | 57 | 0 | PRO L | 8 | | 18.452 | 11.965 | 9.640 | 1.00 | 56.56 | L | 0 |
| | MOTA | 58 50 | | PRO L | 8 | | 21.883 | 12.838 | 9.841 | 1.00 | | L | C |
| | MOTA MOTA | 59 60 | | PRO L | 8 | | 21.358 | 14.219 | 9.760 | 1.00 | | L | C |
| | MOTA | 61 | | ALA L | 8 9 | | 20.911 19.905 | 14.323 11.341 | 8.317 11.244 | $1.00 \\ 1.00$ | | L | C |
| 65 | ATOM | 62 | | ALA L | 9 | | 18.883 | 11.033 | 12.244 12.215 | 1.00 | | L L | C |
| | MOTA | 63 | С | ALA L | 9 | | 18.728 | 12.221 | 13.136 | 1.00 | | L | C |
| | MOTA | 64 | | ALA L | 9 | | 17.619 | 12.564 | 13.539 | 1.00 | 34.10 | L | ŏ |
| | MOTA | 65 | CB | ALA L | 9 | | 19.289 | 9.824 | 12.993 | 1.00 | 36.31 | L | Ċ |

| | N | | | | | | | | | | |
|----|------|----------|-------------|---------|----|--------|----------------------|-----------------|------------|--------------------|--------|
| | ATOM | 66 | N | SER L | 10 | 19.856 | 12.841 | 13.471 | 1.00 33.73 | L | N |
| | MOTA | 67 | CA | SER L | 10 | 19.885 | 14.006 | 14.345 | 1.00 34.21 | L | С |
| | ATOM | 68 | C | SER L | 10 | 20.660 | 15.103 | 13.656 | 1.00 30.61 | L | C |
| | MOTA | 69 | 0 | SER L | 10 | 21.478 | 14.840 | 12.786 | 1.00 37.19 | L | 0 |
| 5 | ATOM | 70 | CB | SER L | 10 | 20.562 | 13.673 | 15.663 | 1.00 39.85 | $oldsymbol{r}$ | C |
| • | ATOM | 71 | OG | SER L | 10 | 19.863 | 12.647 | 16.323 | 1.00 58.43 | L | 0 |
| | ATOM | 72 | N | LEU L | 11 | 20.428 | 16.335 | 14.069 | 1.00 29.18 | L | N |
| | ATOM | 73 | CA | LEU L | 11 | 21.094 | 17.449 | 13.441 | 1.00 29.44 | L | C |
| | | 74 74 | C | LEU L | 11 | 21.199 | 18.558 | 14.468 | 1.00 34.45 | L | C |
| • | MOTA | | | LEU L | 11 | 20.206 | 18.914 | 15.099 | 1.00 38.49 | L L | ō |
| 0 | ATOM | 75 | O | | 11 | 20.245 | 17.919 | 12.270 | 1.00 38.78 | L | Č |
| | MOTA | 76 | CB | LEU L | | 20.243 | 19.031 | 11.368 | 1.00 34.38 | L | č |
| | ATOM | 77 | CG | LEU L | 11 | | 18.572 | 10.671 | 1.00 54.90 | L | Č |
| | MOTA | 78 | | | 11 | 22.005 | | | 1.00 34.90 | r L | C |
| | ATOM | 79 | | rea r | 11 | 19.669 | 19.346 | 10.345 | | r r | И |
| 15 | MOTA | 80 | N | ALA L | 12 | 22.394 | 19.110 | 14.643 | 1.00 39.63 | | |
| | ATOM | 81 | $^{\rm CA}$ | ALA L | 12 | 22.798 | 20.159 | 15.575 | 1.00 36.46 | Ĩ | C |
| | MOTA | 82 | C | ALA L | 12 | 23.247 | 21.418 | 14.832 | 1.00 35.24 | r L | C |
| | MOTA | 83 | 0 | ALA L | 12 | 24.322 | 21.485 | 14.251 | 1.00 40.47 | L | 0 |
| | MOTA | 84 | CB | ALA L | 12 | 23.946 | 19.620 | 16.429 | 1.00 39.40 | L | C |
| 20 | MOTA | 85 | N | VAL L | 13 | 22.357 | 22.428 | 14.831 | 1.00 33.94 | L | N |
| | ATOM | 86 | CA | VAL L | 13 | 22.652 | 23.673 | 14.132 | 1.00 44.79 | L | C |
| | MOTA | 87 | C | VAL L | 13 | 22.485 | 24.889 | 15.047 | 1.00 43.03 | L | C |
| | ATOM | 88 | O | VAL L | 13 | 21.747 | 24.879 | 16.023 | 1.00 42.07 | $oldsymbol{T}$ | 0 |
| | ATOM | 89 | CB | VAL L | 13 | 21.698 | 23.787 | 12.942 | 1.00 42.44 | $\mathbf L$ | C |
| 25 | ATOM | 90 | | VAL L | 13 | 21.877 | 25.143 | 12.258 | 1.00 42.25 | L | C |
| 20 | MOTA | 91 | | VAL L | 13 | 21.977 | 22 ⁻ .680 | 11.942 | 1.00 56.66 | ${f r}$ | С |
| | ATOM | 92 | N | SER L | 14 | 23.242 | 25.953 | 14.719 | 1.00 46.49 | L | N |
| | ATOM | 93 | CA | SER L | 14 | 23.145 | 27.177 | 15.505 | 1.00 50.99 | L | C |
| | | 94 | C | SER L | 14 | 22.219 | 28.196 | 14.839 | 1.00 46.51 | L | С |
| 20 | MOTA | 95 | ŏ | SER L | 14 | 22.091 | 28.269 | 13.624 | 1.00 51.52 | L | 0 |
| 30 | ATOM | 96 | - | SER L | 14 | 24.549 | 27.765 | 15.650 | 1.00 51.18 | L | Ċ |
| | ATOM | | CB | | 14 | 25.514 | 26.791 | 15.246 | 1.00 60.81 | Ĺ | ō |
| | ATOM | 97 | OG | SER L | 15 | 21.527 | 28.976 | 15.688 | 1.00 41.47 | L | Ŋ |
| | MOTA | 98 | N | LEU L | | 20.600 | 29.971 | 15.160 | 1.00 43.66 | - L | Ĉ |
| | ATOM | 99 | CA | LEU L | 15 | | 30.669 | 13.918 | 1.00 43.12 | Ŀ | č |
| 35 | ATOM | 100 | C | LEU L | 15 | 21.164 | 30.953 | 13.816 | 1.00 50.89 | L | õ |
| | MOTA | 101 | 0_ | LEU L | 15 | 22.350 | | | 1.00 45.45 | L | ç |
| | ATOM | 102 | CB | LEU L | 15 | 20.325 | 30.998 | 16.261 17.394 | 1.00 45.45 | r. | Č |
| | MOTA | 103 | CG | LEU L | 15 | 19.470 | 30.425 | | | L | č |
| | ATOM | 104 | | LEU L | 15 | 19.079 | 31.484 | 18.428 | 1.00 50.28 | | |
| 40 | MOTA | 105 | | LEU L | 15 | 18.162 | 29.810 | 16.896 | 1.00 48.82 | L | C N |
| | ATOM | 106 | N | GLY L | 16 | 20.308 | 31.017 | 12.967 | 1.00 39.34 | ŗ | |
| | MOTA | . 107 | CA | GLY L | 16 | 20.763 | 31.757 | 11.807 | 1.00 37.83 | $ar{	extbf{L}}$ | C |
| | ATOM | 108 | С | GLY L | 16 | 21.510 | 30.955 | 10.764 | 1.00 36.32 | Ŀ | C |
| | MOTA | 109 | 0 | GLY L | 16 | 21.802 | 31.473 | 9.683 | 1.00 45.28 | $	ilde{	extbf{r}}$ | 0 |
| 45 | ATOM | 110 | N | GLN L | 17 | 21.826 | 29.702 | 11.068 | 1.00 30.61 | Ľ | N |
| | MOTA | 111 | CA | GLN L | 17 | 22.537 | 28.872 | 10.111 | 1.00 33.76 | L | C |
| | MOTA | 112 | C | GLN L | 17 | 21.545 | 28.158 | 9.215 | 1.00 32.65 | L | Ċ |
| | MOTA | 113 | 0 | GLN L | 17 | 20.361 | 28.471 | 9.220 | 1.00 33.30 | L | 0 |
| | MOTA | 114 | CB | GLN L | 17 | 23.417 | 27.851 | 10.833 | 1.00 34.75 | L | С |
| 50 | ATOM | 115 | CG | GLN L | 17 | 24.397 | 28.480 | 11.798 | 1.00 50.05 | L | C |
| | MOTA | 116 | CD | GLN L | 17 | 25.314 | 29.478 | 11.117 | 1.00 50.98 | L | C |
| | ATOM | 117 | OE1 | | 17 | 25.594 | 30.556 | 11.658 | 1.00 48.45 | \mathbf{L} | 0 |
| | ATOM | 118 | NE2 | | 17 | 25.793 | 29.125 | 9.927 | 1.00 32.88 | L | N |
| | ATOM | 119 | N | ARG L | 18 | 22.034 | 27.197 | 8.440 | 1.00 34.50 | L | N |
| 55 | MOTA | 120 | CA | ARG L | 18 | 21.179 | 26.442 | 7.543 | 1.00 29.75 | L | C |
| 33 | MOTA | 121 | C | ARG L | 18 | 21.281 | 24.969 | 7.864 | 1.00 33.92 | L | C |
| | ATOM | 122 | Ö | ARG L | 18 | 22.350 | 24.464 | 8.186 | 1.00 40.96 | L | 0 |
| | | 123 | CB | ARG L | 18 | 21.586 | 26.678 | 6.094 | 1.00 32.75 | L | C |
| | MOTA | | | | 18 | 20.989 | 25.701 | 5.105 | 1.00 27.81 | L | Č |
| 00 | ATOM | 124 | CG | ARG L | | 21.450 | 26.041 | 3.706 | 1.00 37.23 | L | Ċ |
| 60 | MOTA | 125 | CD | ARG L | 18 | 22.909 | 26.054 | 3.700 | 1.00 56.95 | L | Ŋ |
| | ATOM | 126 | NE | ARG L | 18 | | | 2.488 | 1.00 52.86 | Ĺ | Ĉ |
| | MOTA | 127 | CZ | ARG L | 18 | 23.569 | 26.457 | | 1.00 48.42 | L | N |
| | MOTA | 128 | | L ARG L | 18 | 22.909 | 26.891 | 1.419 | 1.00 46.42 | L | N |
| | MOTA | 129 | | ARG L | | 24.898 | 26.415 | 2.465 | | | |
| 65 | MOTA | 130 | N | ALA L | | 20.148 | 24.287 | 7.787 | 1.00 34.89 | L | N |
| | MOTA | 131 | CA | ALA L | | 20.080 | 22.869 | 8.054 | 1.00 31.86 | L | C |
| | MOTA | 132 | C | ALA L | | 19.525 | | 6.799 | 1.00 32.59 | L, | C |
| | ATOM | 133 | 0 | ALA L | | 18.621 | | 6.185 | 1.00 37.78 | Ŀ | 0 |
| | MOTA | 134 | CB | ALA L | 19 | 19.156 | 22.605 | 9.222 | 1.00 26.13 | L | С |

| | ATOM ATOM ATOM | 135 136 137 | CA C | THR L THR L THR L | 20 20 20 | 20.074 19.577 19.269 | 21.093 20.410 18.979 | 6.405 5.228 5.602 | 1.00 36.27 1.00 41.54 1.00 44.55 | L L | С С И |
|----|----------------------|-------------------|------------|-------------------------|---|----------------------------|----------------------------|-------------------------|--|--------|-------------|
| | MOTA | 138 | 0 | THR L | 20 | 20.070 | 18.313 | 6.237 | 1.00 58.65 | L | 0 |
| 5 | MOTA MOTA | 139 140 | CB OG1 | THR L | 20 20 | 20.595 20.875 | 20.402 21.745 | 4.063 3.657 | 1.00 39.53 1.00 50.92 | L L | C |
| | ATOM | 141 | CG2 | THR L | 20 | 20.021 | 19.672 | 2.874 | 1.00 37.47 | L | С |
| | MOTA MOTA | 142 143 | N CA | ILE L ILE L | 21 21 | 18.090 17.700 | 18.512 17.151 | 5.222 5.516 | 1.00 45.42 1.00 38.44 | L L | N C |
| 10 | MOTA | 144 | С | ILE L | 21 | 17.582 | 16.407 | 4.195 | 1.00 38.28 | L | C |
| | ATOM ATOM | 145 146 | O CB | ILE L ILE L | 21 21 | 17.236 16.348 | 16.989 17.103 | 3.157 6.291 | 1.00 39.74 1.00 43.11 | L L | 0 |
| | MOTA | 147 | CG1 | ILE L | 21 | 16.521 | 17.747 | 7.666 | 1.00 44.22 | L | C |
| 15 | ATOM ATOM | 148 149 | CG2 CD1 | ILE L | 21 21 | 15.886 15.320 | 15.653 17.550 | 6.483 8.582 | 1.00 47.73 1.00 56.67 | L L | C C |
| 15 | ATOM | 150 | И | SER L | 22 | 17.885 | 15.115 | 4.251 | 1.00 33.33 | L | N |
| | ATOM ATOM | 151 152 | CA C | SER L SER L | 22 22 | 17.834 16.856 | 14.257 13.114 | 3.083 3.290 | 1.00 32.47 1.00 27.07 | L L | C |
| | ATOM | 153 | Ö | SER L | 22 | 16.629 | 12.685 | 4.419 | 1.00 27.07 | Ľ | 0 |
| 20 | ATOM | 154 | CB | SER L | 22 22 | 19.235 19.185 | 13.703 12.604 | 2.783 1.886 | 1.00 30.96 1.00 38.42 | L L | C |
| | ATOM ATOM | 155 156 | OG N | SER L CYS L | 23 | 16.278 | 12.604 | 2.184 | 1.00 38.42 | L | И |
| | ATOM | 157 | CA | CYS L | 23 | 15.327 15.568 | 11.538 10.763 | 2.177 0.892 | 1.00 32.07 1.00 33.68 | L L | C |
| 25 | ATOM ATOM | 158 159 | C O | CYS L | 23 23 | 15.552 | 11.328 | -0.198 | 1.00 33.68 | L | Ö |
| | ATOM | 160 | CB | CYS L | 23 | 13.881 | 12.066 | 2.201 | 1.00 34.20 | L | C |
| | MOTA MOTA | 161 162 | SG N | CYS L LYS L | 23 24 | 12.480 15.838 | 10.881 9.473 | $2.134 \\ 1.021$ | 1.00 42.49 1.00 32.63 | L L | S N |
| 00 | ATOM | 163 | CA | LYS L | 24 | 16.029 | 8.646 | -0.154 | 1.00 35.47 | L | C |
| 30 | ATOM ATOM | 164 165 | C | LYS L LYS L | $\begin{array}{c} 24 \\ 24 \end{array}$ | 14.977 14.765 | 7.548 6.858 | -0.163 0.839 | 1.00 38.09 1.00 41.45 | L L | C |
| | MOTA | 166 | CB | LYS L | 24 | 17.431 | 8.040 | -0.184 | 1.00 39.20 | L | C |
| | ATOM ATOM | 167. 168 | CG CD | LYS L LYS L | 24 24 | 18.489 18.571 | 8.954 10.293 | -0.787 -0.064 | 1.00 58.69 1.00 73.72 | L L | C C |
| 35 | MOTA | 169 | CE | LYS L | 24 | 19.889 | 11.004 | -0.356 | 1.00 82.49 | L | C |
| | ATOM ATOM | 170 171 | NZ N | LYS L ALA L | 24 25 | 21.089 14.308 | $10.292 \\ 7.409$ | 0.216 -1.298 | 1.00 65.38 1.00 34.05 | L | N |
| | MOTA | 172 | CA | ALA L | 25 | 13.275 | 6.407 | -1.455 | 1.00 36.52 | L | C |
| 40 | ATOM ATOM | 173 174 | C O | ALA L ALA L | 25 25 | 13.775 14.534 | 5.221 5.379 | -2.274 -3.224 | 1.00 37.06 1.00 40.67 | L L | C O |
| .0 | MOTA | 175 | CB | ALA L | 25 | 12.049 | 7.023 | -2.121 | 1.00 32.09 | L | C |
| | ATOM ATOM | 176 177 | N CA | SER L SER L | 26 26 | 13.334 13.698 | $4.034 \\ 2.804$ | -1.886 -2.556 | 1.00 36.30 1.00 39.67 | L L | G M |
| | MOTA | 178 | C | SER L | 26 | 13.130 | 2.728 | -3.973 | 1.00 44.72 | L | C |
| 45 | ATOM ATOM | 179 180 | O CB | SER L SER L | 26 26 | 13.625 13.165 | 1.969 1.630 | -4.798 -1.756 | 1.00 51.00 1.00 45.86 | L L | 0 |
| | MOTA | 181 | OG | SER L | 26 | 11.749 | 1.670 | -1.717 | 1.00 46.37 | L | ŏ |
| | MOTA MOTA | 182 183 | N CA | GLU L | 27 27 | 12.088 11.449 | 3.508 3.510 | -4.248 -5.562 | 1.00 42.93 1.00 36.19 | L L | C |
| 50 | ATOM | 184 | C | GLU L | 27 | 11.029 | 4.915 | -5.964 | 1.00 35.89 | L | С |
| | MOTA MOTA | 185 186 | O CB | GLU L GLU L | 27 27 | 10.712 10.215 | 5.737 2.602 | -5.113 -5.549 | 1.00 44.15 1.00 33.03 | L L | C |
| | MOTA | 187 | CG | GLU L | 27 | 10.513 | 1.112 | -5.429 | 1.00 38.92 | L | С |
| 55 | ATOM ATOM | 188 189 | CD OE1 | GLU L | 27 27 | 9.253 8.952 | $0.263 \\ -0.214$ | -5.329 -4.217 | 1.00 34.14 1.00 56.00 | L L | C |
| 33 | MOTA | 190 | OE2 | | 27 | 8.556 | 0.070 | -6.354 | 1.00 49.04 | L | 0 |
| | ATOM ATOM | 191 192 | N CA | SER L SER L | 28 28 | 11.016 10.659 | 5.184 6.527 | -7.266 -7.708 | 1.00 42.57 1.00 44.76 | L L | С И |
| | ATOM | 193 | CA | SER L | 28 | 9.234 | 6.901 | -7.290 | 1.00 49.62 | L | C |
| 60 | ATOM | 194 | O | SER L | 28 28 | 8.288 10.784 | 6.144 6.578 | -7.465 -9.232 | 1.00 45.16 1.00 45.04 | L L | C |
| | ATOM ATOM | 195 196 | CB OG | SER L SER L | 28 | 10.814 | 7.940 | -9.657 | 1.00 43.90 | L | Ö |
| | MOTA | 197 | N | VAL L | 29 | 9.161 | 8.098 | -6.720 | 1.00 51.26 | L | N |
| 65 | ATOM ATOM | 198 199 | CA C | VAL L VAL L | 29 29 | 7.875 7.302 | 8.643 9.645 | -6.291 -7.303 | 1.00 48.35 1.00 49.03 | L L | C C |
| | MOTA | 200 | 0 | VAL L | 29 | 6.536 | 10.541 | -6.971 | 1.00 53.81 | L | 0 |
| | MOTA MOTA | 201 202 | CB CG1 | VAL L | 29 29 | 8.080 8.959 | 9.339 8.479 | -4.945 -4.041 | 1.00 45.09 1.00 45.73 | L L | C |
| | ATOM | 203 | | VAL L | 29 | 8.743 | 10.687 | -5.153 | 1.00 39.01 | L | C |

| | ATOM | 204 | N | ASP L | 30 | | .725 | 9.490 10.482 | -8.572 -9.561 | 1.00 50.49 1.00 51.89 | L L | N C |
|-----|--------------|-------------------|------------|----------------|------------|---|----------------|------------------|--------------------|--------------------------|----------|--------|
| | ATOM ATOM | 205 206 | CA C | ASP L ASP L | 30 30 | | .314 | | -10.314 | 1.00 55.22 | L L | C |
| | ATOM | 207 | Õ | ASP L | 30 | | .895 | | -10.735 | 1.00 56.81 | L | 0 |
| 5 | MOTA | 208 | CB | ASP L | 30 | | .466 | | -10.547 | 1.00 58.57 | Ŀ | C |
| | ATOM | 209 | CG | ASP L | 30 | | .368 | | -10.050 | 1.00 71.03 1.00 85.53 | L | C |
| | MOTA | 210 | | ASP L ASP L | 30 30 | | .806 .613 | 12.590 11.864 | -10.882 -8.849 | 1.00 85.55 | L L | 0 |
| | MOTA MOTA | $\frac{211}{212}$ | N N | ASP L | 30A | | .107 | 11.007 | | 1.00 62.31 | L | N |
| 10 | ATOM | 213 | CA | ASN L | 30A | | .880 | | -11.174 | 1.00 66.21 | L | C |
| | MOTA | 214 | C | ASN L | 30A | | .739 | | -12.440 | 1.00 72.19 | L | C |
| | MOTA | 215 | 0 | ASN L | 30A | | .151 | | -12.450 | 1.00 71.91 | L | 0 |
| | ATOM | 216 | CB | ASN L ASN L | 30A 30A | | .684 .425 | | -10.255 -10.956 | 1.00 71.89 1.00 77.18 | L L | C |
| 15 | ATOM ATOM | 217 218 | CG OD1 | ASN L | 30A | | .716 | | -11.583 | 1.00 79.23 | L | ŏ |
| 13 | ATOM | 219 | | ASN L | 30A | | .172 | | -10.878 | 1.00 82.39 | L | N |
| | MOTA | 220 | N | TYR L | 30B | | .340 | | -13.532 | 1.00 79.09 | L | N |
| | ATOM | 221 | CA | TYR L | 30B | | .180 | | -14.806 | 1.00 84.64 | L L | C |
| 00 | ATOM | 222 | C | TYR L TYR L | 30B 30B | | .879 .403 | | -14.807 -15.380 | 1.00 80.89 1.00 78.21 | L L | C |
| 20 | ATOM ATOM | 223 224 | O CB | TYR L | 30B | | .684 | | -15.066 | 1.00 92.55 | L | Č |
| | ATOM | 225 | CG | TYR L | 30B | | .049 | | -15.306 | 1.00106.94 | L | C |
| | MOTA | 226 | CD1 | | 30B | _ | .960 | | -14.270 | 1.00124.67 | Ŀ | C |
| | MOTA | 227 | CD2 | | 30B | | .530 | | -16.562 | 1.00117.46 | L | C |
| 25 | ATOM | 228 229 | CE1 CE2 | | 30B 30B | | .349 | | -14.482 -16.777 | 1.00130.56 1.00130.84 | L L | C |
| | MOTA MOTA | 230 | CEZ | TYR L | 30B | | .839 | | -15.744 | 1.00132.90 | L | č |
| | ATOM | 231 | OH | TYR L | 30B | | .224 | | -15.945 | 1.00133.30 | L | 0 |
| | MOTA | 232 | N | GLY L | 30C | | .015 | | -14.087 | 1.00 77.39 | L | N |
| 30 | ATOM | 233 | CA | GLY L | 30C | | 790 | 14.419 15.119 | -14.111 -12.749 | 1.00 76.49 1.00 75.11 | L L | C |
| | ATOM ATOM | 234 235 | C | GLY L | 30C 30C | | .823 .533 | 16.093 | -12.749 | 1.00 77.11 | L L | Ö |
| | ATOM | 236 | N | LYS L | 30D | | .991 | | -11.818 | 1.00 67.87 | L | N |
| | MOTA | 237 | CA | LYS L | 30D | | .920 | 15.263 | -10.510 | 1.00 58.91 | L | C |
| 35 | ATOM | 238 | C | LYS L | 30D | | .254 | 14.295 | -9.367 | 1.00 54.18 | Ŀ | C |
| | ATOM | 239 | 0 | LYS L | 30D | | .840 L.509 | 13.143 15.831 | -9.350 -10.333 | 1.00 53.39 1.00 59.26 | L L | C |
| | ATOM ATOM | $\frac{240}{241}$ | CB CG | LYS L LYS L | 30D 30D | | 1.209 | 16.960 | -10.333 -11.324 | 1.00 53.20 | L | č |
| | ATOM | 242 | CD | LYS L | 30D | | 3.211 | 17.978 | -10.767 | 1.00 82.67 | L | C |
| 40 | ATOM | 243 | CE | LYS L | 30D | 3 | 3.066 | 19.212 | -11.664 | 1.00 98.60 | L | C |
| | ATOM | 244 | NZ | LYS L | 30D | | 2.785 | | -13.035 | 1.00108.42 | Ŀ | N |
| | ATOM | 245 | N | SER L | 31 | | 7.027 | 14.777 13.961 | -8.402 -7.261 | 1.00 48.70 1.00 48.64 | L L | N C |
| | ATOM ATOM | 246 247 | CA C | SER L SER L | 31 31 | | 7.420 5.407 | 14.075 | -6.127 | 1.00 46.46 | L | C |
| 45 | ATOM | 248 | Ö | SER L | 31 | | 5.195 | 15.156 | -5.571 | 1.00 46.13 | L | 0 |
| | ATOM | 249 | CB | SER L | 31 | | 3.798 | 14.391 | -6.760 | 1.00 44.76 | L | C |
| | MOTA | 250 | OG | SER L | 31 | | 734 | 14.408 | -7.818 | 1.00 48.15 | L | O |
| | MOTA | 251 | N | LEU L LEU L | 32 32 | | 5.777 1.796 | 12.956 12.950 | -5.788 -4.717 | 1.00 40.47 1.00 36.96 | L L | C N |
| 50 | MOTA MOTA | 252 253 | CA C | LEU L | 32 | 5 | 5.501 | 12.689 | -3.393 | 1.00 38.57 | L | Č |
| 00 | ATOM | 254 | ŏ | LEU L | 32 | | 5.338 | 11.645 | -2.772 | 1.00 40.41 | L | 0 |
| | MOTA | 255 | CB | LEU L | 32 | | 3.734 | 11.895 | -5.002 | 1.00 37.94 | Ļ | C |
| | ATOM | 256 | CG | LEU L | 32 | | 3.205 | 12.103 11.241 | -6.424 -6.665 | 1.00 38.09 1.00 40.08 | L L | C |
| 55 | MOTA MOTA | 257 258 | | LEU L | 32 32 | | L.975 2.883 | 13.574 | -6.625 | 1.00 40.00 | r L | c |
| 55 | ATOM | 259 | N | MET L | 33 | | 5.288 | 13.675 | -2.982 | 1.00 39.42 | L | N |
| | MOTA | 260 | CA | MET L | 33 | 7 | 7.069 | 13.631 | -1.756 | 1.00 35.69 | L | C |
| | MOTA | 261 | C | MET L | 33 | | 5.618 | 14.837 | -0.949 | 1.00 36.17 | Γ | C |
| 00 | ATOM | 262 | 0 | MET L | 33 | | 5.480 | 15.921 | -1.503 | 1.00 39.26 1.00 35.25 | L L | C |
| 60 | MOTA MOTA | 263 264 | CB CG | MET L MET L | 33 33 | | 3.567 9.519 | 13.741 13.699 | -2.109 -0.937 | 1.00 29.04 | ŗ Ľ | C |
| | MOTA | 265 | SD | MET L | 33 | | 9.186 | 12.324 | 0.219 | 1.00 63.78 | L | S |
| | ATOM | 266 | CE | MET L | 33 | 9 | 9.514 | 10.867 | -0.802 | 1.00 61.41 | L | C |
| . – | ATOM | 267 | N | HIS L | 34 | | 6.383 | 14.659 | 0.347 | 1.00 32.55 | L | N |
| 65 | MOTA | 268 | CA | HIS L | 34 34 | | 5.930 6.689 | 15.773 15.799 | 1.181 2.506 | 1.00 30.96 | L L | C |
| | ATOM ATOM | 269 270 | C O | HIS L HIS L | 34 34 | | 7.011 | 14.747 | 3.052 | 1.00 37.96 | L | ŏ |
| | ATOM | 271 | СВ | HIS L | 34 | 4 | 4.426 | 15.649 | 1.485 | 1.00 31.51 | L | C |
| | MOTA | 272 | CG | HIS L | 34 | : | 3.588 | 15.261 | 0.307 | 1.00 13.71 | L | С |
| | | | | | | | | | | | | |

| | ATOM | 273 | ND1 | HIS L | 34 | 3.397 | 16.087 | -0.780 | 1.00 26.36 | | ь : | ът |
|-------|------|-----|------------------|----------------------------|----|---------|--------|--------|------------|-----|------------|-------------|
| | ATOM | 274 | | HIS L | 34 | 2.882 | | | | | | N |
| | | | | | | | | 0.051 | 1.00 18.42 | | | С |
| | MOTA | 275 | | HIS L | 34 | 2.609 | | -1.654 | 1.00 16.76 |] | L I | С |
| | ATOM | 276 | NE2 | $\mathtt{HIS}\ \mathtt{L}$ | 34 | 2.282 | 14.304 | -1.173 | 1.00 28.77 | Ī | ւ : | N |
| 5 | ATOM | 277 | N | TRP L | 35 | 6.958 | 16.992 | 3.030 | 1.00 30.35 | | | |
| • | ATOM | 278 | | | | | | | | | | N |
| | | | CA | TRP L | 35 | 7.665 | | 4.299 | 1.00 28.13 | | | C |
| | ATOM | 279 | С | TRP L | 35 | 6.826 | 17.615 | 5.487 | 1.00 30.86 |] | Ľ, (| С |
| | MOTA | 280 | 0 | TRP L | 35 | 6.030 | | 5.367 | 1.00 31.74 | | | ō |
| | ATOM | 281 | | TRP L | | 8.877 | | | | | | |
| | | | CB | | 35 | | | 4.145 | 1.00 25.50 |] | | С |
| 10 | ATOM | 282 | CG | TRP L | 35 | 9.953 | 17.475 | 3.293 | 1.00 33.54 |] | L (| C |
| | ATOM | 283 | CD1 | TRP L | 35 | 10.085 | 17.629 | 1.954 | 1.00 22.15 | 7 | ն (| Ċ |
| | MOTA | 284 | CD2 | | 35 | | | | | | | |
| | | | | | | 11.064 | | 3.722 | 1.00 41.05 | | | С |
| | ATOM | 285 | NE1 | TRP L | 35 | 11.211 | 16.981 | 1.513 | 1.00 39.93 |] | L] | N |
| | ATOM | 286 | CE2 | TRP L | 35 | 11.833 | 16.386 | 2.579 | 1.00 39.83 | 7 | | C |
| 15 | ATOM | 287 | CE3 | | 35 | 11.483 | | | | | | |
| 15 | | | | | | | | 4.960 | 1.00 37.32 | | <u>ن</u> (| C |
| | ATOM | 288 | CZ2 | TRP L | 35 | 13.004 | 15.613 | 2.633 | 1.00 34.89 |] | L (| С |
| | ATOM | 289 | CZ3 | TRP L | 35 | 12.648 | 15.406 | 5.010 | 1.00 39.53 | 1 | | С |
| | ATOM | 290 | CH2 | | 35 | 13.391 | 15.134 | | | | | |
| | | | | | | | | 3.856 | 1.00 25.23 | | | С |
| | ATOM | 291 | N | TYR L | 36 | 7.023 | 17.006 | 6.650 | 1.00 26.93 |] | L 1 | N |
| 20 | ATOM | 292 | CA | TYR L | 36 | 6.299 | 17.433 | 7.823 | 1.00 24.56 | 1 | | С |
| | ATOM | 293 | C | TYR L | 36 | 7.218 | | | | | - | \tilde{a} |
| | | | | | | | | 8.968 | 1.00 27.73 | | | C |
| | MOTA | 294 | О | TYR L | 36 | 8.359 | | 9.054 | 1.00 29.41 |] | | 0 |
| | ATOM | 295 | CB | TYR L | 36 | 5.338 | 16.353 | 8.281 | 1.00 27.13 | 1 | . (| С |
| | ATOM | 296 | CG | TYR L | 36 | 4.349 | | 7.222 | 1.00 28.84 | | | Č |
| OF | | | | | | | | | | | | _ |
| 25 | ATOM | 297 | CD1 | | 36 | 4.703 | 15.072 | 6.206 | 1.00 32.70 | 1 | · (| С |
| | ATOM | 298 | CD2 | TYR L | 36 | 3.060 | 16.470 | 7.230 | 1.00 29.19 | 1 | <u> </u> | С |
| | ATOM | 299 | CE1 | TYR L | 36 | 3.800 | 14.706 | 5.233 | 1.00 29.50 | | | Č |
| | | | | | | | | | | | | |
| | MOTA | 300 | CE2 | | 36 | 2.146 | | 6.262 | 1.00 32.05 | . 1 | | С |
| | ATOM | 301 | CZ | TYR L | 36 | 2.516 | 15.230 | 5.269 | 1.00 28.90 | 1 | · (| C |
| 30 | ATOM | 302 | OH | TYR L | 36 | 1.587 | 14.852 | 4.331 | 1.00 31.16 | I | | Ō |
| | ATOM | 303 | | GLN L | 37 | 6.703 | | | | | | |
| | | | N | | | | | 9.832 | 1.00 25.72 | 1 | | N |
| | ATOM | 304 | ca | GLN L | 37 | 7.419 | 19.131 | 11.003 | 1.00 29.42 | I | . (| C |
| | ATOM | 305 | C | GLN L | 37 | 6.540 | 18.825 | 12.198 | 1.00 27.20 | I | | С |
| | ATOM | 306 | Ō | GLN L | 37 | 5.335 | | 12.169 | | | | |
| 05 | | | | | | | | | 1.00 30.38 | | | 0 |
| 35 | ATOM | 307 | CB | GLN L | 37 | 7.671 | 20.633 | 10.950 | 1.00 30.13 | I | · (| C |
| | ATOM | 308 | CG | GLN L | 37 | 8.155 | 21.194 | 12.281 | 1.00 39.28 | I | . (| С |
| | ATOM | 309 | CD | GLN L | 37 | 8.177 | 22.707 | 12.306 | 1.00 36.66 | Ī | | |
| | | | | | | | | | | | | C |
| | ATOM | 310 | OE1 | | 37 | 7.154 | | 12.088 | 1.00 38.84 | I | . (| 0 |
| | ATOM | 311 | NE2 | GLN L | 37 | 9.340 | 23.285 | 12.581 | 1.00 29.96 | I | 5 1 | N |
| 40 | ATOM | 312 | N | GLN L | 38 | 7.145 | | 13.245 | 1.00 27.64 | I | | N |
| | ATOM | 313 | | | | | | | | | | |
| | | | CA | GLN L | 38 | 6.405 | | 14.437 | 1.00 26.94 | I | | С |
| | ATOM | 314 | C | GLN L | 38 | 7.194 | 18.490 | 15.623 | 1.00 27.28 | I | ٠ (| C |
| | MOTA | 315 | 0 | GLN L | 38 | 8.193 | 17.898 | 16.021 | 1.00 29.54 | I | . (| 0 |
| | ATOM | 316 | СB | GLN L | 38 | 6.152 | | | | | | |
| 45 | | | | | | | 16.481 | 14.549 | 1.00 22.51 | I | | C |
| 45 | MOTA | 317 | CG | GLN L | 38 | 5.437 | 16.082 | 15.834 | 1.00 29.24 | I | ٠ (| C |
| | ATOM | 318 | $^{\rm CD}$ | GLN L | 38 | 5.113 | 14.604 | 15.891 | 1.00 29.24 | I | . (| C |
| | ATOM | 319 | OE1 | GLN L | 38 | 5.880 | 13.760 | 15.419 | 1.00 32.49 | Ī | | ŏ |
| | | | NE2 | | | | | | | | | |
| | ATOM | 320 | | | 38 | 3.974 | | 16.486 | 1.00 39.87 | I | | и. |
| | ATOM | 321 | N | LYS L | 39 | 6.737 | 19.614 | 16.166 | 1.00 28.43 | I | . 1 | N |
| 50 | ATOM | 322 | CA | LYS L | 39 | 7.363 | 20.232 | 17.324 | 1.00 26.31 | I | | C |
| | ATOM | 323 | C | LYS L | 39 | 7.019 | | 18.546 | | | | |
| | | | | | | | | | 1.00 31.47 | I | | C |
| | MOTA | 324 | 0 | LYS L | 39 | 5.937 | 18.810 | 18.634 | 1.00 32.57 | I | . (| 0 |
| | ATOM | 325 | $^{\mathtt{CB}}$ | LYS L | 39 | 6.848 | 21.660 | 17.495 | 1.00 25.15 | I | | С |
| | ATOM | 326 | CG | LYS L | 39 | 7.064 | | 16.277 | 1.00 21.42 | | ` } | ă |
| r- r- | | | | | | | | 10.277 | | I | , (| C |
| 55 | MOTA | 327 | $^{\mathrm{CD}}$ | LYS L | 39 | 6.510 | | 16.515 | 1.00 25.95 | Ι | , (| С |
| | ATOM | 328 | CE | LYS L | 39 | 6.913 | 24.841 | 15.418 | 1.00 25.49 | I | | С |
| | ATOM | 329 | NZ | LYS L | 39 | 6.500 | | 15.764 | 1.00 41.94 | | | |
| | | | | | | | | | | I | | N |
| | ATOM | 330 | N | PRO L | 40 | 7.938 | | 19.513 | 1.00 33.67 | I | . 1 | N |
| | ATOM | 331 | CA | PRO L | 40 | 7.732 | 18.575 | 20.737 | 1.00 37.29 | I | | C |
| 60 | ATOM | 332 | C | PRO L | 40 | 6.400 | | 21.429 | 1.00 42.79 | Ī | | |
| 55 | | | | | | | | 01 B01 | | | | C |
| | ATOM | 333 | 0 | PRO L | 40 | 6.055 | 20.011 | 21.724 | 1.00 40.43 | I | | 0 |
| | ATOM | 334 | $^{\mathrm{CB}}$ | PRO L | 40 | 8.939 | 18.950 | 21.587 | 1.00 42.86 | I | | С |
| | ATOM | 335 | CG | PRO L | 40 | 9.983 | 19.257 | 20.560 | 1.00 39.77 | Ī | | C |
| | | | | | | | | | | | | |
| 0.5 | ATOM | 336 | CD | PRO L | 40 | 9.222 | 20.062 | 19.553 | 1.00 29.92 | I | | С |
| 65 | ATOM | 337 | N | GLY L | 41 | 5.648 | 17.790 | 21.668 | 1.00 43.78 | I | . 1 | N |
| | ATOM | 338 | CA | GLY L | 41 | 4.367 | 17.929 | 22.326 | 1.00 46.56 | I | | Ċ |
| | | 339 | | | | | 10 222 | 21 202 | | | | |
| | ATOM | | C | GLY L | 41 | 3.223 | 18.220 | 21.383 | 1.00 43.68 | I | | C |
| | MOTA | 340 | 0 | GLY L | 41 | 2.105 | 18.424 | 21.834 | 1.00 49.55 | I | , (| 0 |
| | ATOM | 341 | N | GLN L | 42 | 3.483 | 18.235 | 20.080 | 1.00 41.00 | I | | N |
| | | | | | | J • ±03 | | | 41.00 | | | |

| | ATOM ATOM | 342 343 | CA C | GLN L | 42 42 | 2.429 | 18.509 17.439 | 19.113 18.031 | 1.00 40.68 1.00 42.38 | L | C |
|---------|--------------|------------|------------|----------------|----------|------------------|------------------|------------------|--------------------------|--------|-----------------|
| | ATOM ATOM | 344 345 | O CB | GLN L GLN L | 42 42 | 2.975 2.674 | 16.410 19.858 | 18.059 18.449 | 1.00 40.20 1.00 44.01 | Ţ. | 0 |
| 5 | ATOM | 346 | CG | GLN L | 42 | 2.908 | 20.997 | 19.419 | 1.00 53.32 | L L | C |
| | MOTA | 347 | CD | GLN L | 42 | 3.214 | 22.303 | 18.716 | 1.00 47.80 | L | Č |
| | MOTA | 348 | OE1 | | 42 | 3.430 | 23.330 | 19.351 | 1.00 82.52 | L | ŏ |
| | ATOM | 349 | NE2 | | 42 | 3.234 | 22.267 | 17.387 | 1.00 57.98 | L | N |
| 40 | ATOM | 350 | N | SER L | 43 | 1.420 | 17.689 | 17.071 | 1.00 41.14 | L | N |
| 10 | ATOM | 351 352 | CA | SER L | 43 | 1.211 | 16.757 | 15.972 | 1.00 42.56 | Ŀ | C |
| | ATOM ATOM | 353 | C | SER L SER L | 43 43 | 1.930 2.415 | 17.230 18.359 | 14.710 14.633 | 1.00 40.84 1.00 43.67 | L | C |
| | ATOM | 354 | СВ | SER L | 43 | -0.280 | 16.509 | 15.699 | 1.00 43.67 | L L | 0 |
| | ATOM | 355 | OG | SER L | 43 | -0.200 | 17.872 | 15.663 | 1.00 40.39 | r L | C |
| 15 | ATOM | 356 | N | PRO L | 44 | 2.018 | 16.367 | 13.702 | 1.00 35.42 | L | Ŋ |
| | ATOM | 357 | CA | PRO L | 44 | 2.705 | 16.792 | 12,484 | 1.00 36.10 | Ē | Ĉ |
| | MOTA | 358 | C | PRO L | 44 | 2.094 | 18.026 | 11.826 | 1.00 33.06 | L | C |
| | ATOM | 359 | 0_ | PRO L | 44 | 0.923 | 18.322 | 12.007 | 1.00 41.89 | L | 0 |
| 20 | ATOM | 360 | CB | PRO L | 44 | 2.623 | 15.550 | 11.601 | 1.00 34.17 | Ŀ | C |
| 20 | ATOM ATOM | 361 362 | CG CD | PRO L PRO L | 44 44 | $2.704 \\ 1.734$ | 14.448 | 12.595 | 1.00 33.70 | L | C |
| | ATOM | 363 | И | LYS L | 45 | 2.912 | 14.925 18.747 | 13.662 11.071 | 1.00 33.48 1.00 37.41 | L L | C |
| | ATOM | 364 | CA | LYS L | 45 | 2.661 | 20.000 | 10.405 | 1.00 37.41 | r L | N C |
| | ATOM | 365 | C | LYS L | 45 | 3.136 | 19.899 | 8.972 | 1.00 36.14 | L | Č |
| 25 | ATOM | 366 | 0 | LYS L | 45 | 4.278 | 19.559 | 8.691 | 1.00 43.37 | L | ŏ |
| | ATOM | 367 | CB | LYS L | 45 | 3.438 | 21.096 | 11.136 | 1.00 36.87 | L | С |
| | ATOM | 368 | CG | LYS L | 45 | 2.712 | 22.442 | 11.101 | 1.00 30.75 | L | С |
| | ATOM ATOM | 369 370 | CD | LYS L LYS L | 45 45 | 3.574 | 23.580 | 11.651 | 1.00 63.53 | Ŀ | C |
| 30 | ATOM | 371 | NZ | LYS L | 45 45 | 2.736 3.328 | 24.707 25.128 | 12.264 13.533 | 1.00 73.22 | L | C |
| 00 | ATOM | 372 | N | LEU L | 46 | 2.387 | 20.252 | 7.929 | 1.00 86.98 1.00 38.47 | L L | N N |
| | ATOM | 373 | ĈA | LEU L | 46 | 2.905 | 20.250 | 6.558 | 1.00 30.47 | r L | C |
| | MOTA | 374 | C | LEU L | 46 | 3.715 | 21.512 | 6.282 | 1.00 27.56 | Ŀ | C |
| | ATOM | 375 | 0 | LEU L | 46 | 3.325 | 22.604 | 6.679 | 1.00 30.41 | L | ō |
| 35 | ATOM | 376 | CB | LEU L | 46 | 1.745 | 20.151 | 5.561 | 1.00 30.51 | L | C |
| | ATOM | 377 | CG | LEU L | 46 | 2.062 | 20.048 | 4.063 | 1.00 32.20 | L | C |
| | MOTA MOTA | 378 379 | | LEU L LEU L | 46 | 2.843 | 18.751 | 3.752 | 1.00 33.50 | Ŀ | C |
| | ATOM | 380 | N N | LEU L | 46 47 | $0.750 \\ 4.848$ | 20.068 21.354 | 3.305 | 1.00 23.20 | L | C |
| 40 | ATOM | 381 | CA | LEU L | 47 | 5.721 | 22.482 | 5.610 5.288 | 1.00 28.53 1.00 28.04 | L L | N C |
| | ATOM | 382 | C | LEU L | 47 | 5.890 | 22.620 | 3.776 | 1.00 28.70 | L | C |
| | MOTA | 383 | 0 | LEU L | 47 | 5.701 | 23.694 | 3.195 | 1.00 29.81 | L | ŏ |
| | ATOM | 384 | CB | LEU L | 47 | 7.100 | 22.267 | 5.894 | 1.00 25.65 | L | Ĉ |
| 45 | ATOM | 385 | CG | LEU L | 47 | 7.289 | 21.941 | 7.367 | 1.00 27.87 | L | С |
| 45 | ATOM | 386 | CD1 | | 47 | 8.738 | 21.534 | 7.578 | 1.00 38.37 | L | C |
| | ATOM ATOM | 387 388 | CD2 N | LEU L ILE L | 47 48 | 6.923 6.274 | 23.136 21.517 | 8.223 3.148 | 1.00 32.83 | L T | C |
| | MOTA | 389 | CA | ILE L | 48 | 6.479 | 21.499 | 1.716 | 1.00 28.34 1.00 27.51 | L L | N N |
| | ATOM | 390 | C | ILE L | 48 | 5.664 | 20.340 | 1.225 | 1.00 26.97 | L | C |
| 50 | MOTA | 391 | 0 | ILE L | 48 | 5.583 | 19.325 | 1.916 | 1.00 23.95 | L | ŏ |
| | MOTA | 392 | CB | ILE L | 48 | 7.981 | 21.227 | 1.336 | 1.00 30.58 | L | C |
| | ATOM | 393 | | ILE L | 48 | 8.896 | 22.342 | 1.865 | 1.00 16.40 | L | C |
| | MOTA | 394 | CG2 | | 48 | 8.112 | 21.058 | -0.173 | 1.00 30.40 | L | С |
| 55 | ATOM ATOM | 395 396 | N | ILE L TYR L | 48 49 | 8.731 | 23.661 | 1.216 | 1.00 27.58 | Ŀ | C |
| 00 | ATOM | 397 | CA | TYR L | 49 | 5.047 4.260 | 20.499 19.424 | 0.052 -0.568 | 1.00 26.36 1.00 28.37 | L L | И |
| | ATOM | 398 | C | TYR L | 49 | 4.706 | 19.327 | -2.021 | 1.00 28.37 | r r | C |
| | ATOM | 399 | ō | TYR L | 49 | 5.155 | 20.318 | -2.604 | 1.00 27.84 | L | õ |
| | MOTA | 400 | CB | TYR L | 49 | 2.752 | 19.692 | -0.488 | 1.00 26.55 | L | Č |
| 60 | ATOM | 401 | CG | TYR L | 49 | 2.286 | 20.901 | -1.257 | 1.00 28.05 | L | C |
| | ATOM | 402 | CD1 | | 49 | 1.996 | 20.824 | -2.614 | 1.00 26.50 | L | C |
| | MOTA | 403 | CD2 | | 49 | 2.134 | 22.127 | -0.625 | 1.00 31.29 | L | C |
| | ATOM | 404 | CE1 CE2 | | 49 | 1.570 | 21.921 | -3.308 | 1.00 9.37 | Ŀ | C |
| 65 | ATOM ATOM | 405 406 | CEZ | TYR L TYR L | 49 49 | $1.711 \\ 1.429$ | 23.225 23.121 | -1.317 | 1.00 22.71 | L r | C |
| | ATOM | 407 | OH | TYR L | 49 | 1.429 | 23.121 24.244 | -2.656 -3.339 | 1.00 21.56 1.00 29.15 | L L | C |
| | ATOM | 408 | N | ARG L | 50 | 4.586 | 18.121 | -2.580 | 1.00 29.13 | L | <i>1</i> 1 O |
| | MOTA | 409 | CA | ARG L | 50 | 4.996 | 17.807 | -3.944 | 1.00 31.83 | L | C |
| | ATOM | 410 | C | ARG L | 50 | 6.452 | 18.210 | -4.163 | 1.00 30.16 | L | č |

| ATOM 411 O ARG L 50 | | | | | | | | | | | | |
|--|---|------|-----|-----|-------|----|--------|--------|---------|------------|----|---|
| ATOM 414 CD ANG L 50 2.570 18.007 -6.937 1.00 38.86 L C C ANG L 15 NO ANG L 50 2.570 18.007 -7.6937 1.00 42.11 L C C ATOM 415 NE ANG L 50 2.570 18.007 -7.6937 1.00 42.11 L C C ATOM 415 NE ANG L 50 1.632 19.209 -7.664 1.00 47.83 L N A ATOM 414 N.12 NE ANG L 50 1.632 19.209 -7.664 1.00 47.783 L L C C ATOM 418 NE ANG L 50 1.632 19.209 -7.666 1.00 57.85 L L C C ATOM 418 NE ANG L 50 1.632 19.209 -7.666 1.00 57.85 L L C C ATOM 419 N ALA L 51 1.736 17.735 -3.278 1.00 59.09 L L N ATOM 419 N ALA L 51 1.736 17.735 -3.278 1.00 59.09 L C C ATOM 420 CA ALA L 51 9.225 19.452 -3.079 1.00 24.07 L N ATOM 421 C ALA L 51 9.225 19.452 -3.079 1.00 24.07 L N ATOM 421 C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C C ALA L 51 9.225 19.452 19.452 19.452 10.00 32.99 L C C ALA L 51 9.225 19.452 19.45 | | MOTA | 411 | 0 | ARG L | 50 | 6.785 | 18.943 | -5.091 | 1.00 36.35 | L | 0 |
| ATOM 415 CD ARG L 50 | | MOTA | 412 | CB | ARG L | 50 | 4.075 | 18.489 | ~4.965 | 1.00 35.34 | L | C |
| ATOM | | MOTA | 413 | CG | ARG L | 50 | 3.869 | 17.654 | -6.233 | 1.00 38.86 | L | |
| 5 ATOM 415 NE ARG L 50 | | | | | | | | | | | | |
| ATOM 416 CZ ARG L 50 1.635 20.202 -7.586 1.00 61.81 L C AROM 417 NH ARG L 50 0.058 19.948 -6.929 1.00 75.42 L N ATOM 418 NH2 ARG L 50 1.777 21.357 -8.225 1.00 59.09 L L N ATOM 418 NH2 ARG L 51 7.316 17.773 -8.225 1.00 59.09 L C N ATOM 419 N ALA L 51 7.316 17.773 -8.225 1.00 24.07 L N ATOM 420 CA ALA L 51 18.33 18.031 -3.357 1.00 24.07 L N ATOM 421 CA ALA L 51 19.226 19.00 19.00 10.00 22.30 L C ALA L 51 19.226 19.00 1 | = | | | | | | | | | | | |
| ATOM 417 NH1 ARG L 50 0 0.508 19.948 -6.929 1.00 75.42 L N ATOM 419 N ALA L 50 17.77 21.357 -8.225 1.00 59.09 L N ATOM 419 N ALA L 51 7.316 17.735 -8.225 1.00 59.09 L N ATOM 421 C ALA L 51 1.7.316 17.735 18.019 -3.357 1.00 26.078 L N ATOM 421 C ALA L 51 1.875 18.019 -3.357 1.00 26.078 L C ATOM 421 C ALA L 51 1.9.235 18.019 -3.357 1.00 32.99 L C ATOM 421 C ALA L 51 1.9.235 19.452 -3.078 1.00 32.99 L C ATOM 422 C ALA L 51 1.9.235 19.452 -3.078 1.00 32.99 L C ATOM 424 C ALA L 51 1.9.235 19.452 -3.358 1.00 32.99 L C ATOM 425 C A SER L 52 1.9.24 19.521 -3.346 1.00 32.30 L C ATOM 424 C S ER L 52 1.9.24 19.521 -3.346 1.00 32.30 L C ATOM 425 C S ER L 52 1.9.24 19.521 -3.346 1.00 32.30 L C ATOM 426 C SER L 52 8.177 22.306 -3.194 1.00 31.91 L C ATOM 427 O SER L 52 8.177 23.006 -3.194 1.00 31.91 L C ATOM 428 C S SER L 52 10.106 22.167 -4.422 1.00 31.84 L C ATOM 429 C S SER L 52 10.106 22.167 -4.422 1.00 31.84 L C ATOM 429 C S SER L 52 9.479 22.322 -5.677 1.00 37.85 L C ATOM 430 N ASN L 53 6.906 22.760 -2.779 1.00 32.30 L C ATOM 431 C ASN L 53 5.790 32.3222 -5.677 1.00 32.30 L C ATOM 432 C ASN L 53 5.790 32.3222 -5.677 1.00 32.30 L C ATOM 433 C ASN L 53 5.790 32.3222 -5.677 1.00 37.85 L C ATOM 435 C ASN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 436 C ASN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 437 NDZ ASN L 53 4.596 23.255 -3.100 10.00 24.55 L C ATOM 438 C B SSN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 430 C B SSN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 430 C B SSN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 430 C B SSN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 437 NDZ ASN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 440 C LEU L 54 4.596 23.255 -4.622 1.00 19.61 L C ATOM 440 C LEU L 54 4.596 23.255 -3.10 1.00 23.59 L N ATOM 440 C LEU L 54 4.596 23.255 -3.10 1.00 23.59 L N ATOM 440 C LEU L 54 4.596 23.255 -3.10 1.00 23.59 L N ATOM 440 C LEU L 54 4.596 23.255 -3.10 1.00 32.70 L C ATOM 440 C C LEU L 54 54 5.650 25.916 1.00 32.70 L C ATOM 445 C G G G G G G G G G G G G G G G G G G | 3 | | | | | | | | | | | |
| ATOM 418 MHZ ARG L 50 | | | | | | | | | | | | |
| ARTOM 419 N ALA L 51 7, 316 17,735 -3.278 1.00 24.07 L N | | | | | | | | | | | | |
| AROM A210 CA ALA L 51 S. 735 18.019 -3.357 1.00 26.98 L C AROM A22 C ALA L 51 10.230 19.621 -2.383 1.00 32.99 L C AROM A22 C ALA L 51 10.230 19.621 -2.383 1.00 32.33 L C AROM A24 N SER L 52 8.560 20.483 -3.600 1.00 32.360 L C AROM A25 C C SER L 52 8.560 20.483 -3.600 1.00 32.36 L C AROM A26 C SER L 52 8.167 32.004 21.10 32.36 L C AROM A26 C SER L 52 8.167 32.004 21.10 32.36 L C AROM A26 C SER L 52 8.167 32.004 21.10 32.36 L C AROM A27 C SER L 52 8.167 32.004 21.10 32.33 L C AROM A27 C SER L 52 20.106 22.126 -3.195 1.00 34.91 L C AROM A27 C AROM A29 OG SER L 52 20.106 22.126 -3.195 1.00 34.91 L C AROM A31 C AROM A31 C AROM L 53 5.944 23.3838 -2.609 1.00 24.50 L C AROM A32 C AROM L 53 5.944 23.3838 -2.609 1.00 24.50 L C AROM A35 C AROM L 53 5.620 23.362 -0.289 1.00 24.50 L C AROM A35 C AROM L 53 5.620 23.362 -0.289 1.00 24.50 L C AROM A35 C AROM L 53 4.586 23.255 -4.622 1.00 19.61 L C AROM A36 C AROM A35 C AROM A35 C AROM A35 C AROM A36 C AROM A37 C AROM A37 C AROM A38 R AROM A37 C AROM A38 R AROM A38 R AROM A38 R AROM A38 R AROM A39 R AROM A39 R AROM A30 | | | | | | | | | | | | |
| ATOM 421 C | | MOTA | 419 | N | ALA L | 51 | | | | | L | |
| ATOM 421 C ALA L 51 9.225 19.452 -3.079 1.00 32.99 L C ATOM 423 CO ALA L 51 19.230 19.621 -2.383 1.00 32.33 L CO ATOM 424 N SER L 52 9.084 17.566 -4.698 1.00 23.60 L C ATOM 425 CA SER L 52 9.084 21.821 -3.346 1.00 32.36 L N ATOM 425 CA SER L 52 9.084 21.821 -3.346 1.00 33.41 L C ATOM 426 C SER L 52 9.084 21.821 -3.346 1.00 33.41 L C ATOM 427 C SER L 52 8.572 21.37 24.391 1.00 34.94 L C ATOM 427 C SER L 52 8.572 21.37 24.391 1.00 34.34 L C ATOM 428 C SER L 52 8.572 21.37 24.391 1.00 34.394 L C ATOM 428 C SER L 52 8.572 21.37 24.391 1.00 34.394 L C ATOM 429 C SER L 52 9.084 21.821 -3.436 1.00 34.394 L C ATOM 429 C SER L 52 9.094 21.821 -3.433 1.00 34.394 L C ATOM 429 C SER L 52 9.094 21.821 2.00 -2.779 1.00 32.30 L N ATOM 420 C A ASN L 53 5.791 24.229 -1.513 1.00 34.394 L C ATOM 420 C A ASN L 53 5.791 24.229 -1.513 1.00 34.394 L C ATOM 421 C A ASN L 53 5.791 24.229 -1.153 1.00 24.50 L C ATOM 431 C A ASN L 53 5.791 24.229 -1.153 1.00 24.50 L C ATOM 431 C A ASN L 53 5.791 24.229 -1.153 1.00 24.50 L C ATOM 434 C B ASN L 53 4.602 23.395 -3.140 1.00 33.31 L C C ATOM 435 C ASN L 53 4.602 23.395 -3.140 1.00 33.31 L C C ATOM 435 ND ASN L 53 4.602 23.395 -3.140 1.00 33.31 L C C ATOM 435 ND ASN L 53 4.602 23.395 -3.140 1.00 33.31 L C C ATOM 437 ND ASN L 53 4.408 24.233 -5.336 1.00 39.42 L C ATOM 438 N L 53 4.408 24.233 -5.336 1.00 39.42 L C ATOM 438 N L SEU L 54 5.839 25.525 -0.869 1.00 23.59 L N ATOM 430 C ALBU L 54 5.839 25.525 -0.869 1.00 37.53 L C C ATOM 430 C ALBU L 54 5.839 25.525 -0.869 1.00 37.53 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 33.33 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 33.23 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 31.23 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 31.23 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 31.23 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 31.23 L C C ATOM 440 C LBU L 54 5.839 25.525 -0.869 1.00 31.23 L C C ATOM 445 C C C C C C C C C C C C C C C C C C |) | MOTA | 420 | CA | ALA L | 51 | 8.735 | 18.019 | -3.357 | 1.00 26.98 | L | C |
| ATOM | | MOTA | | С | ALA L | 51 | 9.225 | 19.452 | -3.079 | 1.00 32.99 | L | C |
| APPOIN | | | | | | | | | -2.383 | | L | |
| ATOM | | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | |
| ATOM 426 C SER L 52 8.137 23.006 -3.194 1.00 31.91 L C O ATOM 427 O SER L 52 10.106 22.167 -4.422 1.00 34.94 L C O ATOM 428 CB SER L 52 10.106 22.167 -4.422 1.00 34.94 L C O ATOM 429 CG SER L 52 9.479 22.322 -5.677 1.00 37.85 L C O ATOM 430 N ASN L 53 6.906 22.760 -2.779 1.00 32.30 L N ATOM 431 CA ASN L 53 5.944 23.838 -2.609 1.00 24.50 L C ATOM 432 C ASN L 53 5.944 23.838 -2.609 1.00 24.50 L C ATOM 433 C ASN L 53 5.620 23.362 -0.289 1.00 37.53 L C ATOM 434 CB ASN L 53 5.620 23.362 -0.289 1.00 37.53 L C ATOM 435 CG ASN L 53 4.602 23.395 -3.140 1.00 13.31 L C ATOM 436 ODL ASN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 437 NDZ ASN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 438 N LEU L 54 5.839 25.525 -0.869 1.00 23.59 L N ATOM 439 N LEU L 54 5.630 25.916 0.519 1.00 19.73 L C ATOM 440 C LEU L 54 4.169 25.939 0.896 1.00 23.59 L N ATOM 440 C LEU L 54 4.169 25.939 0.896 1.00 31.23 L C ATOM 441 C LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 442 CB LEU L 54 6.253 27.310 0.700 1.00 11.00 11.46 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 11.00 11.46 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 11.00 11.46 L C ATOM 445 CG LEU L 54 6.595 2.266 291 3.065 1.00 32.59 L N ATOM 446 N GLU L 55 3.840 25.195 1.906 30.60 2.20 L C ATOM 447 CD LEU L 54 6.253 27.310 0.700 1.00 11.00 11.46 L C ATOM 448 C CD LEU L 54 6.595 2.266 2.210 1.00 32.59 L C ATOM 445 C CD LEU L 54 6.595 2.266 2.210 1.00 32.59 L C ATOM 445 C CD LEU L 55 2.260 2.269 1.3065 1.00 32.79 L C ATOM 447 CO LEU L 55 2.260 2.269 2.266 2.206 1.00 32.79 L C ATOM 448 C CD LEU L 55 2.260 2.260 2.206 1.00 32.79 L C ATOM 445 C CD LEU L 55 2.260 2.260 2.206 1.00 32.79 L C ATOM 445 C CD LEU L 55 2.260 2.260 2.206 1.00 32.79 L C ATOM 445 C CD LEU L 55 2.260 2.260 2.260 1.00 32.79 L C ATOM 445 C CD LEU L 55 2.260 2.260 2.260 1.00 32.79 L C ATOM 455 C CD LEU L 55 2.260 2.260 2.260 1.00 32.79 L C ATOM 450 C CD LEU L 55 2.260 2.260 2.260 1.00 32.79 L C ATOM 450 C CD LEU L 55 2.260 2.260 2.260 1.00 32.79 L C ATOM 450 C CD LEU L 55 2.260 2.260 2.260 1.00 32.79 L C ATOM 45 | _ | | | | | | | | | | | |
| ATOM 428 CB SER L 52 10.106 22.167 -4.422 1.00 31.84 L C C ATOM 429 OG SER L 52 10.106 22.167 -4.422 1.00 31.84 L C C ATOM 430 N ASN L 53 6.906 22.322 -5.677 1.00 37.85 L O ATOM 431 CA ASN L 53 6.906 22.322 -5.677 1.00 37.85 L O ATOM 431 CA ASN L 53 5.944 23.838 -2.609 1.00 24.50 L C ATOM 432 C ASN L 53 5.944 23.838 -2.609 1.00 24.50 L C ATOM 433 O ASN L 53 5.942 22.92 -1.153 1.00 32.30 L N ATOM 433 O ASN L 53 5.942 22.92 -1.153 1.00 32.30 L N ATOM 433 O ASN L 53 5.942 22.94 22.9 -1.153 1.00 37.53 L O ATOM 435 CG ASN L 53 4.602 23.355 -3.140 1.00 37.53 L O ATOM 435 CG ASN L 53 4.602 23.355 -3.140 1.00 37.53 L O ATOM 435 CG ASN L 53 4.602 23.355 -3.140 1.00 37.53 L O ATOM 435 CG ASN L 53 4.506 23.255 -4.622 1.00 19.61 L C ATOM 437 ND2 ASN L 53 4.813 22.040 -5.110 1.00 13.31 L C ATOM 438 N LEU L 54 54 5.636 25.935 0.395 1.00 39.42 L O ATOM 437 ND2 ASN L 53 4.813 22.040 -5.110 1.00 18.53 L N ATOM 439 CA LEU L 54 5.636 25.935 0.396 1.00 13.79 L N ATOM 440 C LEU L 54 5.636 25.935 0.396 1.00 13.79 L N ATOM 440 C LEU L 54 6.253 27.310 0.242 1.00 13.23 L N ATOM 442 CB LEU L 54 6.253 27.310 0.242 1.00 13.46 L C ATOM 444 CD1 LEU L 54 6.195 27.789 2.150 1.00 10.0 41.6 L C ATOM 444 CD1 LEU L 54 6.195 27.89 2.150 1.00 10.0 41.6 L C ATOM 446 CD2 LEU L 54 6.595 29.256 2.306 1.00 23.59 L C ATOM 447 CD2 LEU L 55 2.450 25.231 2.306 1.00 23.59 L C ATOM 448 CD2 LEU L 55 2.450 25.231 2.379 1.00 10.0 41.6 L C ATOM 449 C CD2 LEU L 55 2.450 25.195 1.966 1.00 32.72 L N ATOM 446 CD2 LEU L 55 2.450 25.195 1.966 1.00 32.72 L N ATOM 447 CD CD2 LEU L 55 2.450 25.231 2.379 1.00 10.0 41.6 L C ATOM 448 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.98 L C C ATOM 449 C CD2 LEU L 55 2.450 25.231 2.379 1.00 33.99 L C C ATOM 450 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.99 L C C ATOM 450 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.99 L C C ATOM 450 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.99 L C C ATOM 450 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.99 L C C ATOM 450 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.99 L C C ATOM 450 CD2 LEU L 55 2.450 25.231 2.379 1.00 33.9 | 2 | | | | | | | | | | | |
| ATOM 428 CB SER L 52 10.106 22.167 -4.422 1.00 31.84 L C C ATOM 430 N ASN L 53 6.906 22.760 -2.779 1.00 32.30 L N ATOM 431 CA ASN L 53 6.906 22.760 -2.779 1.00 32.30 L N ATOM 431 CA ASN L 53 6.906 22.760 -2.779 1.00 32.30 L N ATOM 432 C ASN L 53 5.944 23.838 -2.609 1.00 32.30 L N ATOM 432 C ASN L 53 5.944 23.838 -2.609 1.00 37.53 L C ATOM 433 CA ASN L 53 5.944 23.838 -2.629 1.00 37.53 L C ATOM 435 CC ASN L 53 4.602 23.362 -0.289 1.00 37.53 L C ATOM 435 CC ASN L 53 4.602 23.365 -0.289 1.00 37.53 L C ATOM 435 CC ASN L 53 4.602 23.365 -3.140 1.00 13.31 L C ATOM 436 OD1 ASN L 53 4.602 23.365 -3.140 1.00 19.61 L C ATOM 437 ND2 ASN L 53 4.813 22.040 -5.110 1.00 19.61 L C ATOM 437 ND2 ASN L 53 4.813 22.040 -5.110 1.00 19.63 L N ATOM 438 N LEU L 54 5.859 25.525 -0.869 1.00 39.42 L O ATOM 440 C LEU L 54 5.859 25.916 0.519 1.00 19.73 L C ATOM 440 C LEU L 54 4.169 25.939 0.896 1.00 39.42 L O ATOM 440 C LEU L 54 4.169 25.939 0.896 1.00 31.23 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 10.01 1.1 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 1.00 10.01 1.1 L C ATOM 445 CD LEU L 54 6.255 2.256 2.256 1.206 1.00 32.72 L N ATOM 446 N GLU L 55 3.860 27.789 1.250 1.00 30.446 L C ATOM 447 CA GLU L 55 3.860 27.789 1.250 1.00 30.559 L C ATOM 448 C C GLU L 55 3.860 25.2531 1.900 30.559 L C ATOM 448 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C ATOM 448 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C ATOM 449 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C ATOM 445 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C C ATOM 445 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C C ATOM 445 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C C ATOM 445 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C C ATOM 445 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C C ATOM 445 C C GLU L 55 5 2.450 25.231 1.900 30.554 L C C ATOM 445 C C GLU L 55 5 2.450 25.231 1 | | | | | | | | | | | | |
| ATOM | | ATOM | | 0 | | | | | | | L | |
| ATOM 431 CA ASIN L 53 6,906 22.760 -2.779 1.00 32.30 L N ATOM 432 C ASIN L 53 5.944 23.838 -2.609 1.00 24.50 L C ATOM 433 O ASIN L 53 5.944 23.838 -2.609 1.00 24.50 L C ATOM 433 O ASIN L 53 5.791 24.229 -1.153 1.00 28.28 L C ATOM 434 CB ASIN L 53 5.620 23.362 -0.289 1.00 37.53 L O ATOM 435 CG ASIN L 53 4.602 23.395 -3.140 1.00 13.31 L C ATOM 436 OD1 ASIN L 53 4.596 23.255 -4.622 1.00 19.61 L C ATOM 437 ND2 ASIN L 53 4.408 24.233 -5.336 1.00 19.61 L C ATOM 438 N LEU L 54 5.839 25.525 -0.869 1.00 39.42 L O ATOM 439 CA LEU L 54 5.839 25.525 -0.869 1.00 19.73 L C ATOM 440 C LEU L 54 5.839 25.525 -0.869 1.00 23.599 L N ATOM 440 C LEU L 54 4.169 25.939 0.896 1.00 31.23 L C ATOM 441 O LEU L 54 4.169 25.939 0.896 1.00 31.23 L C ATOM 444 CD LEU L 54 6.195 27.789 1.800 34.46 L O ATOM 444 CD LEU L 54 6.195 27.789 1.100 10.41 L C ATOM 444 CD LEU L 54 6.253 27.310 0.700 10.01 11.46 L C ATOM 444 CD LEU L 54 6.195 27.789 2.150 1.00 0.04 1 L C ATOM 446 N G LU L 55 2.450 29.256 2.306 1.00 23.599 L N ATOM 446 N GLU L 55 2.450 25.2316 0.700 10.01 1.46 L C ATOM 446 N GLU L 55 2.450 25.2316 0.00 23.599 L C ATOM 446 N GLU L 55 2.450 25.2316 0.00 23.599 L C ATOM 446 N GLU L 55 2.450 25.2316 0.00 23.599 L C ATOM 446 N GLU L 55 2.450 25.2316 0.00 23.599 L C ATOM 446 N GLU L 55 2.450 25.2316 0.00 23.599 L C ATOM 446 N GLU L 55 2.450 25.2316 0.00 23.599 L C ATOM 446 N GLU L 55 2.2450 26.533 1.906 1.00 32.72 L N ATOM 447 CA GLU L 55 2.2450 25.2316 1.00 32.72 L N ATOM 448 C GLU L 55 2.2450 25.2316 1.00 32.72 L N ATOM 447 CA GLU L 55 2.2450 25.231 1.906 1.00 40.41 L C ATOM 450 CB GLU L 55 0.883 24.310 4.148 1.00 40.02 L C ATOM 450 CB GLU L 55 0.883 24.310 4.148 1.00 40.02 L C ATOM 450 CB GLU L 55 0.883 24.310 4.148 1.00 40.02 L C ATOM 450 CB GLU L 55 0.883 24.310 4.148 1.00 40.02 L C ATOM 450 CB GLU L 55 0.2450 2.9450 2.9450 1.00 33.98 L C ATOM 450 CB GLU L 55 0.2450 2.9450 2.9450 1.00 33.99 L C ATOM 450 CB GLU L 55 0.2450 2.9450 1.00 33.99 L C ATOM 450 CB GLU L 55 0.2450 2.9450 1.00 33.99 L C ATOM 450 CB GLU L 55 0.2450 2.9450 1.00 33.99 L | | MOTA | 428 | CB | SER L | 52 | 10.106 | 22.167 | -4.422 | 1.00 31.84 | L | С |
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| ATOM 438 N LEU L 54 5.839 25.525 -0.869 1.00 23.59 L N ATOM 439 CA LEU L 54 5.650 25.916 0.519 1.00 19.73 L C ATOM 440 C LEU L 54 4.169 25.939 0.896 1.00 31.23 L C ATOM 441 O LEU L 54 6.253 27.310 0.700 1.00 31.23 L C ATOM 442 CB LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 443 CG LEU L 54 6.253 27.310 0.700 1.00 11.46 L C ATOM 444 CD1 LEU L 54 7.125 26.991 3.065 1.00 23.59 L C ATOM 445 CD2 LEU L 54 7.125 26.991 3.065 1.00 23.59 L C ATOM 446 N GLU L 55 3.840 25.195 1.966 1.00 23.59 L C ATOM 446 N GLU L 55 3.840 25.195 1.966 1.00 23.59 L C ATOM 448 C GLU L 55 3.840 25.195 1.966 1.00 23.59 L C ATOM 449 O GLU L 55 2.450 25.231 2.379 1.00 36.54 L C ATOM 449 O GLU L 55 2.860 27.482 3.137 1.00 36.54 L C ATOM 449 C GLU L 55 2.860 27.482 3.137 1.00 36.54 L C ATOM 450 CB GLU L 55 0.883 24.310 4.148 1.00 41.62 L C ATOM 451 CG GLU L 55 0.883 24.310 4.148 1.00 41.65 L C ATOM 453 0E1 GLU L 55 0.883 24.310 4.148 1.00 41.65 L C ATOM 453 0E1 GLU L 55 0.096 23.783 3.130 1.00 41.65 L C ATOM 455 0E2 GLU L 55 0.883 24.310 4.148 1.00 41.65 L C ATOM 455 0E2 GLU L 55 0.883 24.310 4.148 1.00 41.65 L C ATOM 455 0E2 GLU L 55 0.148 23.949 1.945 1.00 54.51 L O ATOM 457 0E2 GLU L 55 0.883 24.310 4.148 1.00 41.65 L C ATOM 455 N SER L 56 0.259 28.168 3.253 1.00 61.09 L O ATOM 457 C SER L 56 0.259 28.168 3.246 1.00 47.94 L O ATOM 458 0 SER L 56 0.259 28.168 3.246 1.00 47.94 L O ATOM 457 C SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 459 CB SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 0E3 SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 0E3 SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 0E3 SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 CB SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 CB SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 CB SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 450 CB SER L 56 0.403 27.270 6.405 1.00 37.39 L N ATOM 460 O G SER L 56 0.403 27.270 6.405 1.00 37.39 L N ATOM 460 O G SER L 56 0.403 27.270 6.405 1.00 37.39 L N ATOM 460 O G SER L 56 0.403 27.270 6.406 1.00 37.39 L C ATOM 460 | | | | | | | | | | | | |
| ATOM | | MOTA | 437 | ND2 | ASN L | 53 | 4.813 | | -5.110 | 1.00 18.53 | L | N |
| ATOM | | MOTA | 438 | N | LEU L | 54 | 5.839 | 25.525 | -0.869 | 1.00 23.59 | L | N |
| ATOM | | MOTA | 439 | CA | LEU L | 54 | 5,650 | 25.916 | 0.519 | 1.00 19.73 | L | C |
| ATOM 441 O LEU L 54 3.338 26.555 0.242 1.00 34.46 L O ATOM 442 CB LEU L 54 6.253 27.310 0.700 1.00 10.41 L C ATOM 443 CG LEU L 54 6.195 27.789 2.150 1.00 10.41 L C ATOM 444 CD1 LEU L 54 7.125 26.991 3.065 1.00 23.59 L C ATOM 445 CD2 LEU L 54 6.595 29.256 2.306 1.00 20.82 L C C ATOM 446 N GLU L 55 3.840 25.195 1.966 1.00 32.72 L N ATOM 447 CA GLU L 55 2.450 25.231 2.379 1.00 36.54 L C ATOM 448 C GLU L 55 2.450 25.231 2.379 1.00 36.54 L C ATOM 449 O GLU L 55 2.860 27.482 3.137 1.00 50.477 L O ATOM 449 O GLU L 55 2.860 27.482 3.137 1.00 50.477 L O ATOM 450 CB GLU L 55 2.889 24.273 3.555 1.00 33.98 L C ATOM 450 CB GLU L 55 0.883 24.310 4.148 1.00 41.02 L C ATOM 451 CG GLU L 55 0.883 24.310 4.148 1.00 41.02 L C ATOM 452 CD GLU L 55 0.883 24.310 4.148 1.00 41.02 L C ATOM 453 OB1 GLU L 55 0.148 23.949 1.945 1.00 54.51 L O ATOM 454 OB2 GLU L 55 0.148 23.949 1.945 1.00 54.51 L O ATOM 457 C SER L 56 0.728 26.885 2.752 1.00 48.75 L N ATOM 458 O SER L 56 0.432 28.262 4.758 1.00 41.16 L C ATOM 458 O SER L 56 0.432 28.262 4.758 1.00 47.94 L O ATOM 450 CB SER L 56 0.432 28.262 4.758 1.00 37.97 L C ATOM 459 CB SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 460 OG SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 460 CG SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 460 CG SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 461 N GLY L 57 0.690 29.617 6.733 1.00 37.39 L N ATOM 463 N GLY L 57 0.690 29.617 6.733 1.00 37.39 L N ATOM 464 N GLY L 57 0.690 29.617 6.733 1.00 37.99 L C ATOM 468 O GLY L 57 0.690 29.617 6.733 1.00 38.10 L C ATOM 467 C GLY L 58 5.298 1.288 7 0.00 37.39 L C ATOM 468 O GLY L 57 0.690 29.617 6.733 1.00 38.10 L C ATOM 468 O GLY L 57 0.690 29.584 6.452 1.00 37.39 L N ATOM 468 C GLY L 58 5.298 1.288 7 0.00 37.39 L N ATOM 468 C G LLE L 58 5.298 1.288 7 0.00 37.39 L C ATOM 468 C G LLE L 58 5.298 1.288 7 0.00 37.39 L C ATOM 470 C G LLE L 58 5.298 29.584 6.452 1.00 38.81 L C C ATOM 470 C G LLE L 58 5.298 29.588 6 8.288 1.00 33.81 L C C ATOM 470 C G LLE L 58 5.298 29.588 6 8.288 1.00 33.81 L C C ATOM 470 C C ROL L 59 6. | 0 | | | | | | | | | | | |
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| ATOM 448 C GLU L 55 2.042 26.636 2.808 1.00 44.62 L C ATOM 449 O GLU L 55 2.289 24.273 3.555 1.00 33.98 L C C ATOM 450 CB GLU L 55 2.289 24.273 3.555 1.00 33.98 L C C ATOM 451 CG GLU L 55 0.883 24.310 4.148 1.00 41.02 L C ATOM 452 CD GLU L 55 0.883 24.310 4.148 1.00 41.65 L C ATOM 453 OE1 GLU L 55 0.148 23.949 1.945 1.00 54.51 L O ATOM 454 OE2 GLU L 55 0.148 23.949 1.945 1.00 54.51 L O ATOM 455 N SER L 56 0.728 26.885 2.752 1.00 48.75 L N ATOM 455 N SER L 56 0.259 28.168 3.246 1.00 41.16 L C ATOM 457 C SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 458 O SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 450 OG SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 450 OG SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 450 OG SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 460 OG SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 460 OG SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 460 OG SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 460 N GLY L 57 0.576 29.464 5.298 1.00 37.39 L N ATOM 461 N GLY L 57 0.576 29.464 5.298 1.00 37.39 L N ATOM 462 CA GLY L 57 0.590 29.617 6.733 1.00 37.90 L C ATOM 463 C GLY L 57 2.056 29.256 7.280 1.00 37.90 L C ATOM 466 CA ILLE L 58 2.981 28.867 6.411 1.00 48.99 L O ATOM 466 CA ILLE L 58 2.981 28.867 6.411 1.00 48.99 L O ATOM 468 O ILLE L 58 5.298 29.584 6.452 1.00 36.39 L C ATOM 469 CB ILLE L 58 5.290 29.584 6.452 1.00 36.39 L C ATOM 469 CB ILLE L 58 5.2981 28.867 6.411 1.00 22.67 L C ATOM 470 CG1 ILLE L 58 5.2981 28.867 6.411 1.00 22.67 L C ATOM 471 CG2 ILLE L 58 6.191 26.817 6.745 1.00 23.574 L C ATOM 473 N PRO L 59 6.197 29.974 7.361 1.00 35.74 L N ATOM 474 CA PRO L 59 6.197 29.974 7.361 1.00 35.74 L N ATOM 475 C PRO L 59 8.000 30.700 5.835 1.00 41.02 L C ATOM 476 O PRO L 59 8.000 30.700 5.835 1.00 41.02 L C ATOM 476 C PRO L 59 8.000 30.700 5.835 1.00 41.02 L C ATOM 478 CG PRO L 59 8.000 30.700 5.835 1.00 41.02 L C ATOM 478 CG PRO L 59 8.000 30.700 5.835 1.00 41.02 L C ATOM 478 CG PRO L 59 8.000 30.700 5.835 1.00 41.00 35.70 L C | | ATOM | 447 | CA | GLU L | 55 | 2.450 | 25.231 | 2.379 | 1.00 36.54 | L | С |
| ATOM | | | | | | | | | | | L | |
| ATOM | | | | | | | | | | | | |
| ATOM 451 CG GLU L 55 | ^ | | | | | | | | | | | |
| ATOM 452 CD GLU L 55 -0.096 23.783 3.130 1.00 41.65 L C ATOM 453 OE1 GLU L 55 -1.080 23.168 3.533 1.00 61.09 L O ATOM 454 OE2 GLU L 55 -1.080 23.168 3.533 1.00 61.09 L O ATOM 455 N SER L 56 0.728 26.885 2.752 1.00 48.75 L N ATOM 456 CA SER L 56 0.259 28.168 3.246 1.00 41.16 L C ATOM 457 C SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 458 O SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 459 CB SER L 56 -1.214 28.307 2.875 1.00 40.01 L C ATOM 460 OG SER L 56 -1.453 27.637 1.636 1.00 57.19 L O ATOM 461 N GLY L 57 0.576 29.464 5.298 1.00 37.39 L N ATOM 462 CA GLY L 57 0.690 29.617 6.733 1.00 38.10 L C ATOM 463 C GLY L 57 2.056 29.256 7.280 1.00 37.90 L C ATOM 464 O GLY L 57 2.056 29.256 7.280 1.00 37.90 L C ATOM 465 N ILE L 58 2.981 28.867 6.411 1.00 48.99 L O ATOM 466 CA ILE L 58 4.312 28.507 6.869 1.00 33.29 L C ATOM 467 C ILE L 58 5.290 29.584 6.452 1.00 33.29 L C ATOM 468 O ILE L 58 5.290 29.584 6.452 1.00 33.81 L C ATOM 469 CB ILE L 58 3.809 26.051 6.745 1.00 33.81 L C ATOM 470 CG1 ILE L 58 3.809 26.051 6.745 1.00 22.67 L C ATOM 470 CG1 ILE L 58 3.809 26.051 6.745 1.00 23.54 L C ATOM 471 CG2 ILE L 58 3.809 26.051 6.745 1.00 23.574 L N ATOM 473 N PRO L 59 6.197 29.974 7.361 1.00 35.74 L N ATOM 474 CA PRO L 59 8.000 30.700 5.835 1.00 31.36 L C ATOM 475 C PRO L 59 8.000 30.700 5.835 1.00 31.36 L C ATOM 476 O PRO L 59 8.257 29.530 5.525 1.00 39.78 L O ATOM 476 O PRO L 59 8.107 30.927 8.353 1.00 31.36 L C ATOM 477 CB PRO L 59 8.107 30.927 8.353 1.00 31.36 L C ATOM 476 O PRO L 59 8.257 29.530 5.525 1.00 39.78 L O ATOM 476 O PRO L 59 8.257 29.530 5.525 1.00 39.78 L O ATOM 476 O PRO L 59 8.257 29.530 5.525 1.00 39.78 L O ATOM 477 CB PRO L 59 8.257 29.530 5.525 1.00 39.78 L O ATOM 476 O PRO L 59 8.257 29.530 5.525 1.00 39.78 L O ATOM 477 CB PRO L 59 8.207 30.927 8.353 1.00 31.36 L C | U | | | | | | | | | | | |
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| 5 ATOM 455 N SER L 56 0.728 26.885 2.752 1.00 48.75 L N ATOM 456 CA SER L 56 0.259 28.168 3.246 1.00 41.16 L C ATOM 458 O SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 459 CB SER L 56 -1.214 28.307 2.875 1.00 47.94 L O ATOM 460 OG SER L 56 -1.214 28.307 2.875 1.00 40.01 L C ATOM 461 N GLY L 57 0.576 29.464 5.298 1.00 37.39 L N ATOM 462 CA GLY L 57 2.056 29.526 7.280 1.00 37.90 L C ATOM 465 N < | | ATOM | 453 | OE1 | GLU L | 55 | 0.148 | | | | L | 0 |
| ATOM 456 CA SER L 56 0.259 28.168 3.246 1.00 41.16 L C ATOM 457 C SER L 56 0.432 28.262 4.758 1.00 39.72 L C ATOM 458 O SER L 56 0.403 27.270 5.475 1.00 47.94 L O ATOM 459 CB SER L 56 -1.214 28.307 2.875 1.00 40.01 L C ATOM 460 OG SER L 56 -1.214 28.307 2.875 1.00 40.01 L C ATOM 461 N GLY L 57 0.576 29.464 5.298 1.00 37.39 L N ATOM 461 N GLY L 57 0.690 29.617 6.733 1.00 38.10 L C ATOM 463 C GLY L 57 2.056 29.256 7.280 1.00 37.90 L C ATOM 464 O GLY L 57 2.056 29.256 7.280 1.00 37.90 L C ATOM 465 N LLE L 58 2.981 28.867 6.411 1.00 41.88 L N ATOM 466 CA ILE L 58 4.312 28.507 6.869 1.00 33.29 L C ATOM 468 O ILE L 58 5.290 29.584 6.452 1.00 36.39 L C ATOM 468 O ILE L 58 5.290 29.584 6.452 1.00 36.39 L C ATOM 469 CB ILE L 58 4.761 27.151 6.280 1.00 33.81 L C ATOM 470 CG1 ILE L 58 3.809 26.051 6.745 1.00 40.95 L O ATOM 471 CG2 ILE L 58 3.809 26.051 6.745 1.00 22.67 L C ATOM 472 CD1 ILE L 58 3.785 25.886 8.238 1.00 23.574 L C ATOM 473 C CPRO L 59 8.000 30.700 5.835 1.00 39.78 L C ATOM 474 CA PRO L 59 7.214 31.007 7.114 1.00 37.66 L C ATOM 475 C PRO L 59 8.000 30.700 5.835 1.00 31.36 L C ATOM 476 O PRO L 59 8.257 29.530 5.525 1.00 39.78 L C ATOM 477 CB PRO L 59 8.000 30.700 5.835 1.00 31.36 L C ATOM 477 CB PRO L 59 8.207 30.927 8.355 1.00 31.36 L C ATOM 478 CG PRO L 59 8.207 30.927 8.355 1.00 31.36 L C ATOM 477 CB PRO L 59 8.207 30.927 8.355 1.00 31.36 L C ATOM 478 CG PRO L 59 7.221 30.346 9.394 1.00 35.70 L C | | ATOM | 454 | OE2 | GLU L | 55 | -1.080 | 23.168 | 3.533 | 1.00 61.09 | L | 0 |
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| | ATOM ATOM ATOM ATOM | 481 | N CA C | ALA L ALA L ALA L ALA L | 60 60 60 | 8.393 9.138 10.609 11.470 | 31.736 31.493 31.228 31.852 | 5.095 3.868 4.141 3.546 | 1.00 44.34 1.00 41.55 1.00 39.49 1.00 42.78 | r r | N C C |
|----|--|--|--------------------------------|--|----------------------------|--|--|--|--|-----------------------|-----------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM | | CB N CA C | ALA L ARG L ARG L ARG L ARG L | 60 61 61 61 61 | 8.987 10.892 12.270 12.397 13.152 | 32.655 30.314 29.941 28.428 27.848 | 2.895 5.065 5.350 5.355 6.127 | 1.00 42.73 1.00 41.36 1.00 36.65 1.00 30.32 1.00 32.09 | L L L L | С С С |
| 10 | MOTA MOTA MOTA | 489 490 491 492 | CB CG CD NE | ARG L ARG L ARG L ARG L | 61 61 61 61 | 12.774 11.819 12.451 11.723 11.822 | 30.563 30.552 31.161 30.730 29.512 | 6.664 7.806 9.057 10.249 10.774 | 1.00 35.38 1.00 39.45 1.00 42.92 1.00 55.59 1.00 47.56 | L L L L | C C C |
| 15 | ATOM ATOM ATOM ATOM ATOM | 495 496 497 | NH2 N CA | ARG L ARG L PHE L PHE L | 61 61 62 62 | 12.725 10.997 11.638 11.614 | 28.668 29.127 27.810 26.365 | 10.312 11.734 4.453 4.260 | 1.00 50.56 1.00 51.77 1.00 28.28 1.00 25.29 1.00 22.96 | L L L | N N C C |
| 20 | ATOM ATOM ATOM ATOM ATOM | 498 499 500 501 502 | | PHE L PHE L PHE L PHE L | 62 62 62 62 62 | 11.638 11.133 10.343 10.393 11.066 | 26.072 26.860 25.784 25.672 24.623 | 2.755 1.970 4.883 6.379 6.983 | 1.00 33.28 1.00 31.62 1.00 25.29 1.00 22.72 | L L L | 0 0 0 |
| 25 | ATOM ATOM ATOM ATOM ATOM | 503 504 505 506 507 | CE1 | PHE L PHE L PHE L PHE L SER L | 62 62 62 62 63 | 9.767 11.110 9.809 10.478 12.205 | 26.617 24.526 26.522 25.483 24.953 | 7.182 8.365 8.561 9.154 2.333 | 1.00 24.93 1.00 41.78 1.00 30.52 1.00 23.52 1.00 23.17 | L L L L | C C C N |
| 30 | ATOM ATOM ATOM ATOM | 508 509 510 511 | CA C O CB | SER L SER L SER L SER L | 63 63 63 63 | 12.238 12.633 13.326 13.227 14.579 | 24.676 23.247 22.629 25.617 25.316 | 0.902 0.612 1.402 0.198 0.539 | 1.00 30.22 1.00 27.52 1.00 33.38 1.00 38.88 1.00 46.56 | L L L L | 00000 |
| 35 | MOTA ATOM ATOM MOTA MOTA | 512 513 514 515 516 | OG N CA C | SER L GLY L GLY L GLY L | 64 64 64 | 12.212 12.563 12.896 12.524 | 22.724 21.357 21.134 21.935 | -0.531 -0.861 -2.328 -3.180 | 1.00 24.58 1.00 30.22 1.00 33.27 1.00 36.12 | L L L | N C C O N |
| 40 | ATOM ATOM ATOM ATOM ATOM | 517 518 519 520 521 | N CA C O CB | SER L SER L SER L SER L SER L | 65 65 65 65 | 13.610 13.961 14.327 14.558 15.120 | 19.728 18.256 17.561 | -2.624 -4.000 -4.147 -3.160 -4.487 | 1.00 33.35 1.00 38.52 1.00 36.43 1.00 42.08 1.00 37.34 | L L L L | 0000 |
| 45 | ATOM ATOM ATOM ATOM ATOM ATOM | 522 523 524 525 526 527 | OG N CA C O | SER L GLY L GLY L GLY L GLY L SER L | 65 66 66 66 66 | 16.285 14.366 14.684 13.681 12.821 | 20.339 17.798 16.421 15.847 16.550 | -3.742 -5.395 -5.690 -6.671 -7.178 -6.954 | 1.00 50.72 1.00 33.13 1.00 31.58 1.00 36.03 1.00 37.03 1.00 39.41 | L L L L L | И С О И |
| 50 | ATOM ATOM ATOM ATOM ATOM | 528 529 530 531 532 | CA C O CB OG | SER L SER L SER L SER L SER L | 67 67 67 67 67 | 12.885 13.192 14.104 13.042 14.309 | 13.900 12.420 12.000 14.423 14.105 | -7.855 -7.790 -7.076 -9.284 -9.835 | 1.00 44.59 1.00 49.82 1.00 48.37 1.00 48.35 1.00 56.59 | L L L | 00000 |
| 55 | ATOM ATOM ATOM ATOM ATOM | 533 534 535 536 537 | N CA C O CB | ARG L ARG L ARG L ARG L ARG L | 68 68 68 68 | 12.421 12.605 12.825 11.904 13.806 | 10.183 9.569 9.098 9.887 | -8.531 -8.578 -7.185 -6.533 -9.475 | 1.00 52.66 1.00 54.25 1.00 47.35 1.00 45.82 1.00 61.56 1.00 72.12 | L L L | и с с |
| 60 | MOTA MOTA MOTA MOTA MOTA | 538 539 540 541 542 | CG CD NE CZ NHI | ARG L ARG L ARG L ARG L I ARG L | 68 68 68 68 | 13.389 13.851 14.580 14.440 13.684 | 8.145 7.503 6.171 5.491 | -11.319 -10.223 -10.089 -10.928 | 1.00 89.41 1.00103.03 1.00112.09 1.00118.70 | L L L L | C N C |
| 65 | ATOM ATOM ATOM ATOM ATOM ATOM | 543 544 545 546 547 548 | NH2 N CA C O CB | 2 ARG L THR L THR L THR L THR L THR L | 68 69 69 69 69 | 15.095 14.068 14.349 15.110 15.193 | 9.569 9.946 9.743 9.316 | -4.364 -3.217 | 1.00 40.89 1.00 39.24 | r r r r | и С С С |
| | | | | | | 70 | | | | | |

| | | | | | | 14 | | | | | |
|----|---|------------|------------------|------------------|-----------------|------------------|--------------------|------------------|--------------------------|---------|--------|
| | ATOM | 549 | | 1 THR L | | 16.296 | | -6.375 | 1.00 58.12 | L | 0 |
| | ATOM ATOM | 550 551 | CG: | 2 THR L ASP L | | 14.218 15.678 | | | 1.00 45.58 | L | С |
| | ATOM | 552 | CA | | | 16.414 | | | 1.00 44.06 1.00 44.09 | L | N |
| 5 | MOTA | 553 | С | ASP L | 70 | 15.686 | | | 1.00 42.38 | L L | C |
| | MOTA | 554 | | ASP L | | 15.227 | 13.618 | -4.507 | 1.00 41.69 | L | ŏ |
| | ATOM ATOM | 555 556 | CB CG | ASP L ASP L | | 17.829 | | | 1.00 52.55 | L | C |
| | ATOM | 557 | | L ASP L | | 18.757 19.971 | | -4.248 -4.428 | 1.00 58.23 1.00 72.20 | L | C |
| 10 | ATOM | 558 | | 2 ASP L | | 18.296 | | -4.426 | 1.00 72.20 | L L | 0 |
| | ATOM | 559 | N | PHE L | 71 | 15.599 | 13.417 | -2.286 | 1.00 31.65 | Ľ | N |
| | ATOM ATOM | 560 561 | CA C | PHE L PHE L | 71 | 14.999 | 14.688 | -1.908 | 1.00 28.67 | L | С |
| | MOTA | 562 | 0 | PHE L | 71 71 | 15.713 16.458 | 15.299 14.650 | -0.705 0.018 | 1.00 28.28 | L | C |
| 15 | ATOM | 563 | СВ | PHE L | 71 | 13.526 | | -1.567 | 1.00 33.98 1.00 25.73 | L L | С 0 |
| | ATOM | 564 | CG | PHE L | 71 | 12.839 | 13.782 | -2.718 | 1.00 32.61 | Ŀ | Č |
| | MOTA MOTA | 565 566 | | L PHE L PHE L | 71 71 | 12.658 | 12.404 | -2.703 | 1.00 28.95 | L | С |
| | ATOM | 567 | | l PHE L | 71 | 12.364 11.994 | | -3.776 -3.752 | 1.00 22.54 | L | C |
| 20 | ATOM | 568 | | PHE L | 71 | 11.696 | 13.912 | -4.823 | 1.00 43.28 1.00 33.39 | L L | G |
| | ATOM | 569 | CZ | PHE L | 71 | 11.510 | 12.535 | -4.816 | 1.00 23.28 | L | č |
| | ATOM ATOM | 570 571 | N CA | THR L | 72 | 15.490 | 16.609 | -0.532 | 1.00 23.10 | L | N |
| | ATOM | 572 | CA | THR L | 72 72 | 16.108 15.271 | 17.295 18.488 | $0.591 \\ 1.041$ | 1.00 30.26 1.00 28.38 | L | C |
| 25 | MOTA | 573 | ō | THR L | 72 | 14.699 | 19.228 | 0.249 | 1.00 28.38 | L L | C |
| | ATOM | 574 | CB | THR L | 72 | 17.496 | 17.769 | 0.155 | 1.00 25.36 | Ŀ | č |
| | ATOM ATOM | 575 576 | OG1 CG2 | | 72 | 17.355 | 18.682 | -0.936 | 1.00 51.91 | L | 0 |
| | ATOM | 577 | N CG2 | LEU L | 72 73 | 18.335 15.178 | 16.574 18.634 | -0.303 2.372 | 1.00 41.87 | L | C |
| 30 | MOTA | 578 | CA | LEU L | 73 | 14.474 | 19.780 | 2.920 | 1.00 31.36 1.00 30.10 | L L | C N |
| | ATOM | 579 | C | LEU L | 73 | 15.456 | 20.784 | 3.522 | 1.00 28.13 | L | C |
| | ATOM ATOM | 580 581 | 0 | LEU L | 73 | 16.310 | 20.454 | 4.334 | 1.00 30.08 | L | 0 |
| | ATOM | 582 | CB CG | LEU L | 73 73 | 13.509 13.010 | 19.274 20.393 | 3.996 4.915 | 1.00 37.24 | L | C |
| 35 | ATOM | 583 | | LEU L | 73 | 11.826 | 21.151 | 4.313 | 1.00 24.15 1.00 21.16 | L L | C |
| | MOTA | 584 | | LEU L | 73 | 12.540 | 19.880 | 6.277 | 1.00 25.70 | L | C |
| | ATOM ATOM | 585 586 | N | THR L | 74 | 15.395 | 22.054 | 3.158 | 1.00 34.02 | L | N |
| | ATOM | 587 | CA C | THR L | 74 74 | 16.418 15.816 | 23.013 24.170 | $3.610 \\ 4.400$ | 1.00 29.77 | ŗ | C |
| 40 | ATOM | 588 | ŏ | THR L | $7\overline{4}$ | 14.888 | 24.170 | 3.978 | 1.00 31.14 1.00 43.23 | Ľ L. | C |
| | ATOM | 589 | CB | THR L | 74 | 17.016 | 23.586 | 2.382 | 1.00 29.59 | P. | č |
| | ATOM ATOM | 590 591 | OG1 | THR L | 74 | 17.206 | 22.556 | 1.474 | 1.00 42.71 | L | 0 |
| | ATOM | 592 | N N | ILE L | 74 75 | 18.371 16.364 | $24.266 \\ 24.361$ | 2.641 5.587 | 1.00 10.54 | L | C |
| 45 | ATOM | 593 | CA | ILE L | 75 | 15.775 | 25.436 | 6.333 | 1.00 34.45 1.00 41.45 | L L | C N |
| | ATOM | 594 | C | ILE L | 75 | 16.807 | 26.527 | 6.632 | 1.00 41.83 | L | č |
| | ATOM ATOM | 595 596 | 0 | ILE L | 75 | 17.713 | 26.346 | 7.402 | 1.00 43.17 | ${f L}$ | _ |
| | ATOM | 597 | CB CG1 | ILE L | 75 75 | 15.112 15.596 | 24.818 25.432 | 7.549 8.817 | 1.00 44.27 1.00 44.83 | L | C |
| 50 | MOTA | 598 | CG2 | | 75 | 15.370 | 23.303 | 7.635 | 1.00 49.07 | L L | C |
| | ATOM | 599 | | ILE L | 75 | 14.424 | 25.873 | 9.656 | 1.00 34.16 | ī. | č |
| | $\begin{array}{c} {\tt ATOM} \\ {\tt ATOM} \end{array}$ | 600 601 | N CA | ASN L ASN L | 76 | 16.646 | 27.635 | 5.919 | 1.00 40.24 | L | N |
| | ATOM | 602 | CA | ASN L | 76 76 | 17.489 16.652 | 28.819 30.087 | 5.986 6.164 | 1.00 35.58 | L | C |
| 55 | ATOM | 603 | ŏ | ASN L | 76 | 15.850 | 30.465 | 5.317 | 1.00 39.86 1.00 46.58 | L L | C O |
| | ATOM | 604 | $^{\mathrm{CB}}$ | ASN L | 76 | 18.282 | 28.894 | 4.679 | 1.00 36.33 | L L | č |
| | ATOM | 605 | CG | ASN L | 76 | 19.497 | 29.764 | 4.867 | 1.00 39.90 | L | C |
| | ATOM ATOM | 606 607 | | ASN L ASN L | 76 76 | 19.789 20.225 | 30.248 29.964 | 5.957 3.756 | 1.00 40.70 | L | 0 |
| 60 | ATOM | 608 | N | PRO L | 77 | 16.833 | 30.740 | 7.330 | 1.00 38.22 1.00 38.97 | L L | N |
| | ATOM | 609 | CA | PRO L | 77 | 17.746 | 30.270 | 8.355 | 1.00 42.09 | L | N C |
| | MOTA | 610 611 | C | PRO L | 77 | 17.024 | 29.423 | 9.410 | 1.00 41.44 | L | С |
| | ATOM ATOM | 611 612 | O CB | PRO L PRO L | 77 77 | 15.813 18.294 | 29.239 31.528 | 9.389 9.020 | 1.00 46.26 | L | 0 |
| 65 | MOTA | 613 | CG | PRO L | 77 | 17.252 | 32.636 | 8.840 | 1.00 43.72 1.00 34.23 | L L | C C |
| | ATOM | 614 | CD | PRO L | 77 | 16.244 | 31.990 | 7.769 | 1.00 40.31 | L | C |
| | MOTA | 615 616 | N | VAL L | 78 70 | 17.828 | 28.875 | 10.340 | 1.00 38.94 | L | N |
| | ATOM ATOM | 616 617 | CA C | VAL L VAL L | 78 78 | 17.249 16.892 | 28.098 29.001 | 11.432 | 1.00 32.51 | I. | C |
| | | J , | - | v.iid Li | , 0 | 10.032 | 49.001 | 12.617 | 1.00 37.03 | L | С |

| | ATOM ATOM | 618 619 | O VAL L CB VAL L | 78 78 | 17.467 18.276 | 30.059 27.052 | 12.828 11.871 | 1.00 39.75 1.00 28.69 | L L | 0 C |
|------|--------------|------------|----------------------|----------------|-------------------------|----------------------------|-------------------------|--|---------|-----------------|
| | ATOM | 620 | CG1 VAL L | 78 | 17.923 | 26.534 | 13.267 | 1.00 19.40 | L | C |
| | ATOM | 621 | CG2 VAL L | 78 | 18.292 | 25.890 | 10.894 | 1.00 29.97 | L | C |
| 5 | MOTA | 622 | N GLU L | 79 | 15.874 | 28.566 | 13.386 | 1.00 38.02 | L | N |
| | MOTA | 623 | CA GLU L | 79 | 15.482 | 29.378 | 14.537 | 1.00 27.34 | L L | C |
| | ATOM | 624 | C GLU L | 79 79 | $15.120 \\ 14.910$ | 28.517 27.315 | 15.754 15.657 | 1.00 34.89 1.00 38.06 | L | C O |
| | ATOM | 625 626 | O GLU L CB GLU L | 79 79 | 14.282 | 30.235 | 14.130 | 1.00 16.08 | L | č |
| 10 | ATOM ATOM | 627 | CG GLU L | 79 | 14.702 | 31.568 | 13.507 | 1.00 50.15 | _ L | Č |
| 10 | ATOM | 628 | CD GLU L | 79 | 13.474 | 32.414 | 13.257 | 1.00 65.88 | L | C |
| | ATOM | 629 | OE1 GLU L | 79 | 13.604 | 33.478 | 12.669 | 1.00 80.47 | L | 0 |
| | MOTA | 630 | OE2 GLU L | 79 | 12.388 | 31.997 | 13.658 | 1.00 78.67 | Ŀ | 0 |
| | ATOM | 631 | N ALA L | 80 | 15.115 | 29.190 | 16.923 | 1.00 39.01 | Ē | Ŋ |
| 15 | ATOM | 632 | CA ALA L | 80 | 14.912 | 28.483 | 18.188 | 1.00 34.33 | L | C |
| | ATOM | 633 | C ALA L | 80 | 13.650 | 27.611 26.506 | 18.188 18.717 | 1.00 39.68 1.00 52.15 | L L | 0 |
| | MOTA | 634 | O ALA L CB ALA L | 80 80 | 13.626 14.823 | 29.530 | 19.299 | 1.00 28.88 | r r | Ċ |
| | ATOM ATOM | 635 636 | CB ALA L N ASP L | 81 | 12.588 | 28.135 | 17.590 | 1.00 38.66 | Ī. | N |
| 20 | ATOM | 637 | CA ASP L | 81 | 11.303 | 27.455 | 17.561 | 1.00 40.47 | L | C |
| 20 | ATOM | 638 | C ASP L | 81 | 11.194 | 26.376 | 16.478 | 1.00 36.22 | L | C |
| | ATOM | 639 | O ASP L | 81 | 10.126 | 25.821 | 16.228 | 1.00 41.23 | L | 0 |
| | ATOM | 640 | CB ASP L | 81 | 10.196 | 28.505 | 17.410 | 1.00 42.43 | Ē | C |
| | MOTA | 641 | CG ASP L | 81 | 8.824 | 27.892 | 17.263 | 1.00 57.83 1.00 69.72 | L L | C |
| 25 | ATOM | 642 | OD1 ASP L | 81 | 8.398 8.173 | 27.135 28.172 | $18.170 \\ 16.231$ | 1.00 68.60 | L | Ö |
| | ATOM ATOM | 643 644 | OD2 ASP L N ASP L | 81 82 | 12.305 | 26.064 | 15.838 | 1.00 30.22 | L | Ŋ |
| | ATOM | 645 | CA ASP L | 82 | 12.273 | 25.043 | 14.817 | 1.00 28.43 | L | C |
| | MOTA | 646 | C ASP L | 82 | 12.670 | 23.660 | 15.349 | 1.00 29.30 | L | C |
| 30 | ATOM | 647 | O ASP L | 82 | 12.728 | 22.691 | 14.589 | 1.00 27.94 | L | 0 |
| | MOTA | 648 | CB ASP L | 82 | 13.165 | 25.454 | 13.643 | 1.00 31.74 | Ţ. | C |
| | ATOM | 649 | CG ASP L | 82 | 12.662 | 26.704 | 12.950 | 1.00 31.05 1.00 45.58 | L L | C |
| | ATOM | 650 | OD1 ASP L | 82 | 11.432 | 26.853 27.533 | 12.823 12.521 | 1.00 45.58 | L | 0 |
| O.E. | ATOM | 651 652 | OD2 ASP L N VAL L | 82 83 | 13.488 12.952 | 27.553 | 16.646 | 1.00 28.22 | L | И |
| 35 | MOTA MOTA | 653 | N VAL L CA VAL L | 83 | 13.293 | 22.263 | 17.201 | 1.00 33.72 | L | Ĉ |
| | ATOM | 654 | C VAL L | 83 | 12.097 | 21.348 | 16.997 | 1.00 28.29 | Ŀ | C |
| | MOTA | 655 | O VAL L | 83 | 10.978 | 21.655 | 17.417 | 1.00 20.55 | L | 0 |
| | MOTA | 656 | CB VAL L | 83 | 13.637 | 22.313 | 18.717 | 1.00 34.51 | L | C |
| 40 | MOTA | 657 | CG1 VAL L | 83 | 14.877 | 23.162 | 18.932 | 1.00 57.28 | L | C |
| | ATOM | 658 | CG2 VAL L | 83 | 12.471 | 22.856 | 19.516 16.337 | 1.00 38.24 1.00 27.89 | L L | N |
| | MOTA | 659 | N ALA L | 84 84 | 12.348 11.303 | 20.225 19.274 | 16.033 | 1.00 27.89 | L | Ç |
| | MOTA ATOM | 660 661 | CA ALA L C ALA L | 84 | 11.903 | 18.093 | 15.293 | 1.00 25.39 | L | Ċ |
| 45 | ATOM | 662 | O ALA L | 84 | 13.117 | 18.001 | 15.103 | 1.00 25.68 | L | 0 |
| | MOTA | 663 | CB ALA L | 84 | 10.265 | 19.940 | 15.150 | 1.00 22.54 | L | C |
| | MOTA | 664 | N THR L | 85 | 11.042 | 17.171 | 14.893 | 1.00 34.15 | Ŀ | \widetilde{N} |
| | MOTA | 665 | CA THR L | 85 | 11.492 | 16.045 | 14.104 | 1.00 37.68 | L | C |
| | MOTA | 666 | C THR L | 85 | 10.798 9.630 | 16.295 16.689 | 12.773 12.740 | 1.00 36.49 1.00 36.43 | L L | Ö |
| 50 | ATOM ATOM | 667 668 | O THR L CB THR L | 85 85 | 11.065 | 14.685 | 14.705 | 1.00 36.97 | Ľ | č |
| | ATOM | 669 | OG1 THR L | 85 | 11.703 | 14.518 | 15.974 | 1.00 43.47 | L | Ō |
| | MOTA | 670 | CG2 THR L | 85 | 11.483 | 13.540 | 13.799 | 1.00 18.61 | L | С |
| | ATOM | 671 | N TYR L | 86 | 11.531 | 16.094 | 11.685 | 1.00 29.71 | Ŀ | Ŋ |
| 55 | ATOM | 672 | CA TYR L | 86 | 11.001 | 16.324 | 10.362 | 1.00 19.30 | Ŀ | C |
| | MOTA | 673 | C TYR L | 86 | 10.879 | 15.017 | 9.616 9.588 | 1.00 22.60 1.00 26.94 | L L | C |
| | MOTA | 674 | O TYR L | 86 86 | 11.814 11.917 | 14.226 17.306 | 9.621 | 1.00 20.34 | Ľ | Č |
| | ATOM ATOM | 675 676 | CB TYR L CG TYR L | 86 | 11.931 | 18.678 | 10.264 | 1.00 17.43 | L | Č |
| 60 | MOTA | 677 | CD1 TYR L | 86 | 12.627 | 18.908 | 11.430 | 1.00 9.96 | L | C |
| 50 | ATOM | 678 | CD2 TYR L | 86 | 11.183 | 19.726 | 9.734 | 1.00 18.42 | L | С |
| | ATOM | 679 | CE1 TYR L | 86 | 12.574 | 20.136 | 12.054 | 1.00 25.73 | L | C |
| | ATOM | 680 | CE2 TYR L | 86 | 11.126 | 20.951 | 10.347 | 1.00 10.31 | L | C |
| | MOTA | 681 | CZ TYR L | 86 | 11.823 | 21.153 | 11.509 | 1.00 24.98 1.00 26.22 | L T. | C |
| 65 | 2 00016 | 682 | OH TYR L | 86 | 11.772 | 22.378 | 12.137 | 1.00 40.44 | L | 0 |
| | ATOM | | | 07 | 0 771 | 1/ 707 | 9 012 | 1 00 25 84 | Τ. | N |
| | MOTA | 683 | N TYR L | 87 87 | 9.721 | 14.787 13.550 | 9.012 8.275 | 1.00 25.84 1.00 29.22 | L L | N C |
| | | | | 87 87 87 | 9.721 9.495 9.097 | 14.787 13.550 13.742 | 9.012 8.275 6.828 | 1.00 25.84 1.00 29.22 1.00 29.46 1.00 34.41 | L L | C N |

| | MOTA | 687 | CB TYR L | 87 | 8.370 | 12.715 | 8.897 | 1.00 30.13 | L | С |
|-----|------|-----|-----------|----|--------|--------|--------|------------|-------------------------------|----|
| | ATOM | 688 | CG TYR L | 87 | 8.442 | 12.448 | 10.381 | 1.00 37.49 | L | C |
| | MOTA | 689 | CD1 TYR L | 87 | 8.122 | 13.440 | 11.304 | 1.00 23.56 | $\widetilde{	ilde{	ilde{L}}}$ | č |
| | ATOM | 690 | CD2 TYR L | 87 | 8.755 | 11.180 | | | | Č |
| _ | | | | | | | 10.857 | 1.00 20.61 | L | C |
| 5 | MOTA | 691 | CE1 TYR L | 87 | 8.108 | 13.168 | 12.651 | 1.00 30.25 | L | С |
| | ATOM | 692 | CE2 TYR L | 87 | 8.742 | 10.900 | 12.201 | 1.00 29.15 | L | C |
| | MOTA | 693 | CZ TYR L | 87 | 8.418 | 11.894 | 13.093 | 1.00 38.77 | L L | č |
| | | | | | | | | | | |
| | MOTA | 694 | OH TYR L | 87 | 8.411 | 11.612 | 14.438 | 1.00 53.01 | L | 0 |
| | ATOM | 695 | N CYS L | 88 | 9.646 | 12.909 | 5.949 | 1.00 36.95 | Ŀ | N |
| 10 | MOTA | 696 | CA CYS L | 88 | 9.243 | 12.950 | 4.555 | 1.00 36.03 | L | Ĉ |
| | | | | | | | | | | C |
| | ATOM | 697 | C CYS L | 88 | 8.105 | 11.924 | 4.423 | 1.00 34.89 | L | C |
| | MOTA | 698 | O CYS L | 88 | 7.938 | 11.047 | 5.271 | 1.00 39.85 | L | 0 |
| | MOTA | 699 | CB CYS L | 88 | 10.407 | 12.624 | 3.600 | 1.00 32.83 | L | C |
| | ATOM | 700 | SG CYS L | 88 | 11.475 | 11.173 | 3.916 | 1.00 43.40 | | č |
| | | | | | | | | | L | S |
| 15 | MOTA | 701 | N GLN L | 89 | 7.302 | 12.058 | 3.380 | 1.00 30.65 | ${f L}$ | N |
| | MOTA | 702 | CA GLN L | 89 | 6.192 | 11.151 | 3.167 | 1.00 30.50 | L | C |
| | MOTA | 703 | C GLN L | 89 | 5.920 | 11.109 | 1.675 | 1.00 32.47 | L | č |
| | | | | | | | | | | |
| | MOTA | 704 | O GLN L | 89 | 5.987 | 12.129 | 0.995 | 1.00 32.80 | L | 0 |
| | MOTA | 705 | CB GLN L | 89 | 4.961 | 11.652 | 3.945 | 1.00 30.53 | L | С |
| 20 | ATOM | 706 | CG GLN L | 89 | 3.695 | 10.818 | 3.821 | 1.00 22.52 | L | C |
| | ATOM | 707 | CD GLN L | 89 | 2.779 | 11.312 | 2.724 | 1.00 21.93 | | |
| | | | | | | 77.277 | | | L | C |
| | MOTA | 708 | OE1 GLN L | 89 | 2.455 | 12.494 | 2.670 | 1.00 30.39 | L | 0 |
| | MOTA | 709 | NE2 GLN L | 89 | 2.349 | 10.408 | 1.843 | 1.00 37.87 | L | N |
| | ATOM | 710 | N GLN L | 90 | 5.647 | 9.921 | 1.159 | 1.00 31.97 | L | N |
| 25 | MOTA | 711 | CA GLN L | 90 | 5.364 | | | | | |
| 25 | | | | | | 9.794 | -0.260 | 1.00 38.12 | L | С |
| | MOTA | 712 | C GLN L | 90 | 3.872 | 9.464 | -0.365 | 1.00 39.89 | ${f L}$ | C |
| | MOTA | 713 | O GLN L | 90 | 3.246 | 8.993 | 0.575 | 1.00 41.18 | L | 0 |
| | MOTA | 714 | CB GLN L | 90 | 6.352 | 8.823 | -0.923 | 1.00 31.71 | ī. | č |
| | | | | | | | | | | |
| | MOTA | 715 | CG GLN L | 90 | 6.391 | 7.458 | ~0.303 | 1.00 40.36 | L | C |
| 30 | MOTA | 716 | CD GLN L | 90 | 5.263 | 6.565 | -0.773 | 1.00 39.74 | L | C |
| | MOTA | 717 | OE1 GLN L | 90 | 4.831 | 6.655 | -1.921 | 1.00 36.34 | L | 0 |
| | MOTA | 718 | NE2 GLN L | 90 | 4.765 | 5.711 | 0.116 | 1.00 46.02 | | |
| | | | | | | | | | L | N. |
| | MOTA | 719 | N SER L | 91 | 3.353 | 9.760 | -1.570 | 1.00 36.91 | L | N |
| | MOTA | 720 | CA SER L | 91 | 1.948 | 9.472 | ~1.784 | 1.00 41.30 | L | С |
| 35 | ATOM | 721 | C SER L | 91 | 1.791 | 8.953 | -3.225 | 1.00 39.89 | L | Č |
| 00 | | | | | | | | | | |
| | MOTA | 722 | O SER L | 91 | 0.731 | 9.043 | -3.842 | 1.00 44.63 | L | 0 |
| | MOTA | 723 | CB SER L | 91 | 1.013 | 10.688 | -1.596 | 1.00 40.49 | L | C |
| | ATOM | 724 | OG SER L | 91 | 1.407 | 11.742 | -2.446 | 1.00 44.85 | L | 0 |
| | MOTA | 725 | N ASN L | 92 | 2.877 | 8.390 | ~3.735 | | | |
| 40 | | | | | | | | 1.00 40.08 | L | N |
| 40 | MOTA | 726 | CA ASN L | 92 | 2.896 | 7.879 | -5.091 | 1.00 40.12 | L | С |
| | MOTA | 727 | C ASN L | 92 | 2.465 | 6.427 | ~5.208 | 1.00 41.27 | Ŀ | С |
| | MOTA | 728 | O ASN L | 92 | 1.930 | 6.019 | -6.234 | 1.00 39.94 | L | ō |
| | MOTA | | | | | | | | | |
| | | 729 | CB ASN L | 92 | 4.291 | 8.044 | -5.676 | 1.00 42.77 | \mathbf{L} | C' |
| | MOTA | 730 | CG ASN L | 92 | 4.349 | 7.649 | -7.118 | 1.00 45.02 | L | C |
| 45 | MOTA | 731 | OD1 ASN L | 92 | 3.502 | 8.057 | -7.911 | 1.00 47.49 | L | 0 |
| | MOTA | 732 | ND2 ASN L | 92 | 5.344 | 6.842 | ~7.473 | 1.00 58.39 | Ĺ | |
| | | | | | | | | | | N |
| | MOTA | 733 | N GLU L | 93 | 2.711 | 5.644 | -4.166 | 1.00 41.39 | $\mathbf{L}_{\mathbf{I}}$ | N |
| | MOTA | 734 | CA GLU L | 93 | 2.326 | 4.236 | -4.167 | 1.00 48.66 | L | C |
| | MOTA | 735 | C GLU L | 93 | 1.677 | 3.914 | -2.829 | 1.00 48.42 | L | С |
| 50 | MOTA | 736 | O GLU L | 93 | 1.986 | 4.537 | -1.821 | 1.00 50.64 | Ľ | ŏ |
| - | | | | | | | | | | |
| | MOTA | 737 | CB GLU L | 93 | 3.553 | 3.328 | -4.338 | 1.00 55.59 | L | С |
| | MOTA | 738 | CG GLU L | 93 | 4.476 | 3.649 | -5.515 | 1.00 62.95 | L | C |
| | MOTA | 739 | CD GLU L | 93 | 3.974 | 3.106 | -6.838 | 1.00 78.92 | L | Č |
| | MOTA | 740 | OE1 GLU L | 93 | | | | | | |
| | | | | | 4.737 | 3.164 | -7.832 | 1.00 84.87 | L | 0 |
| 55 | MOTA | 741 | OE2 GLU L | 93 | 2.821 | 2.623 | -6.887 | 1.00 81.56 | L | 0 |
| | MOTA | 742 | N ASP L | 94 | 0.774 | 2.943 | -2.822 | 1.00 49.35 | L | N |
| | MOTA | 743 | CA ASP L | 94 | 0.121 | 2.531 | -1.588 | 1.00 51.37 | | |
| | | | | | | | | | L | C |
| | MOTA | 744 | C ASP L | 94 | 0.883 | 1.323 | -1.053 | 1.00 50.25 | L | C |
| | MOTA | 745 | O ASP L | 94 | 1.332 | 0.473 | -1.823 | 1.00 50.31 | L | 0 |
| 60 | ATOM | 746 | CB ASP L | 94 | -1.334 | 2.158 | -1.856 | 1.00 49.09 | Ĺ | č |
| ~ • | | | CG ASP L | | | | | | | |
| | MOTA | 747 | | 94 | -2.158 | 3.346 | -2.316 | 1.00 69.28 | L | C |
| | MOTA | 748 | OD1 ASP L | 94 | ~1.734 | 4.029 | ~3.280 | 1.00 79.28 | L | 0 |
| | MOTA | 749 | OD2 ASP L | 94 | -3.229 | 3.597 | -1.717 | 1.00 83.48 | L | 0 |
| | MOTA | 750 | N PRO L | 95 | 1.047 | 1.234 | 0.275 | 1.00 46.17 | L | Ŋ |
| 65 | | | | | | | | | | |
| 65 | MOTA | 751 | CA PRO L | 95 | 0.553 | 2.202 | 1.255 | 1.00 45.81 | L | C |
| | MOTA | 752 | C PRO L | 95 | 1.474 | 3.404 | 1.368 | 1.00 44.56 | L | C |
| | MOTA | 753 | O PRO L | 95 | 2.689 | 3.244 | 1.381 | 1.00 49.31 | L | Ō |
| | MOTA | 754 | CB PRO L | 95 | 0.532 | 1.389 | 2.535 | 1.00 49.20 | | |
| | | | | | | | | | L | C |
| | MOTA | 755 | CG PRO L | 95 | 1.764 | 0.558 | 2.379 | 1.00 42.46 | L | С |

| 5 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 756 757 758 759 760 761 | CD N CA C O CB | PRO L TRP L TRP L TRP L TRP L | 95 96 96 96 96 | 1.691 0.898 1.692 2.572 2.085 0.783 | 0.095 4.600 5.814 5.666 5.410 7.032 | 0.950 1.446 1.575 2.798 3.898 1.716 | 1.00 44.07 1.00 39.90 1.00 33.94 1.00 32.06 1.00 34.49 1.00 33.74 | L L L L L | C N C C O C |
|-----|--------------------------------------|--|-------------------------------|---|----------------------------|--|--|--|--|-----------------------|----------------------------|
| 10 | ATOM ATOM ATOM ATOM ATOM | 762 763 764 765 766 | CG | TRP L TRP L TRP L TRP L TRP L | 96 96 96 96 96 | 0.087 0.093 -0.764 -0.702 -1.239 | 7.384 6.667 8.515 7.273 8.411 | 0.438 -0.717 0.202 -1.654 -1.115 | 1.00 40.68 1.00 32.69 1.00 45.95 1.00 35.93 1.00 35.73 | L L L L | С С С |
| 15 | ATOM ATOM ATOM ATOM | 767 768 769 770 | CE3 CZ2 CZ3 CH2 | TRP L TRP L TRP L TRP L | 96 96 96 96 | -1.169 -2.094 -2.022 -2.473 | 9.605 9.346 10.538 10.401 | 0.978 -1.674 0.416 -0.897 | 1.00 46.81 1.00 44.57 1.00 41.43 1.00 42.28 | L L L L | ממממ |
| 10 | ATOM ATOM ATOM ATOM | 771 772 773 774 | N CA C | THR L THR L THR L THR L | 97 97 97 97 | 3.874 4.810 5.530 5.689 | 5.830 5.661 6.928 7.888 | 2.605 3.702 4.159 3.400 | 1.00 22.72 1.00 20.77 1.00 25.09 1.00 34.55 | L L L | N C C O |
| 20 | ATOM ATOM ATOM ATOM | 775 776 777 778 | CB OG1 CG2 N | THR L | 97 97 97 98 | 5.821 6.443 5.123 5.934 | 4.568 4.876 3.263 6.931 | 3.350 2.106 3.179 5.423 | 1.00 12.22 1.00 27.43 1.00 16.82 1.00 23.17 | L L L | C C N |
| 25 | ATOM ATOM ATOM ATOM | 779 780 781 782 | CA C O CB | PHE L PHE L PHE L | 98 98 98 98 | 6.630 8.092 8.446 6.026 | 8.067 7.744 6.612 8.457 | 6.002 6.256 6.588 7.350 | 1.00 26.77 1.00 34.08 1.00 40.23 1.00 26.01 | L L L L | 0000 |
| 30 | ATOM ATOM ATOM | 783 784 785 786 | CD2 CE1 | PHE L PHE L PHE L | 98 98 98 98 | 4.716 3.546 4.648 2.331 | 9.169 8.471 10.534 9.109 11.192 | 7.263 7.010 7.506 7.009 7.506 | 1.00 23.16 1.00 21.59 1.00 22.33 1.00 17.66 1.00 30.19 | L L L | מטטט |
| 35 | ATOM ATOM ATOM | 787 788 789 790 | CE2 CZ N CA | PHE L GLY L GLY L | 98 98 99 99 | 3.428 2.263 8.944 10.346 10.449 | 10.476 8.748 8.532 8.396 | 7.260 6.112 6.389 7.895 | 1.00 36.03 1.00 37.98 1.00 37.48 1.00 34.91 | L L L | C N C |
| | MOTA MOTA ATOM ATOM | 791 792 793 794 | C O N CA | GLY L GLY L GLY L | 99 99 100 100 | 9.557 11.532 11.726 11.894 | 8.831 7.792 7.594 8.862 | 8.622 8.362 9.784 10.587 | 1.00 38.68 1.00 36.84 1.00 36.30 1.00 34.70 | L L L | О И С |
| 40 | MOTA MOTA MOTA | 795 796 797 798 | C N CA | GLY L GLY L GLY L | 100 101 101 | 11.850 12.096 12.244 | 8.808 9.993 11.267 11.761 | 11.809 9.914 10.611 10.964 | 1.00 37.11 1.00 37.37 1.00 34.43 1.00 31.97 | L L L L | O N C |
| 45 | ATOM ATOM ATOM ATOM | 799 800 801 802 803 | C N CA C | GLY L GLY L THR L THR L THR L | 101 102 102 | 13.650 14.584 13.809 15.099 14.966 | 10.981 13.075 13.630 14.643 | 11.156 11.045 11.447 12.590 | 1.00 31.95 1.00 26.36 1.00 26.88 1.00 33.12 | L L L L | 0 N C |
| 50 | ATOM ATOM ATOM ATOM ATOM | 804 805 806 807 | O CB OG1 CG2 | THR L THR L THR L | 102 102 102 | 14.243 15.736 16.027 17.044 | 15.628 14.302 13.300 14.985 | 12.513 10.231 9.256 10.641 | 1.00 43.00 1.00 27.40 1.00 42.19 1.00 27.02 | L L L | 0 0 0 |
| 55 | ATOM ATOM ATOM ATOM | 808 809 810 811 | N CA O | LYS L LYS L LYS L LYS L | 103 103 103 103 | 15.680 15.643 16.573 17.748 | 14.344 15.234 16.435 16.307 | 13.691 14.845 14.655 14.345 | 1.00 34.75 1.00 37.63 1.00 34.36 1.00 42.52 | L L L L | и С С |
| 60 | ATOM MOTA ATOM ATOM | 812 813 814 815 | CB CG CD CE | LYS L LYS L LYS L | 103 103 103 | 16.069 14.997 15.610 14.873 | 14.433 14.419 14.460 13.561 | 16.075 17.165 18.567 19.566 | 1.00 39.61 1.00 60.51 1.00 81.15 1.00 89.92 1.00 87.84 | L L L L | Z C C C Z |
| 0.5 | ATOM ATOM ATOM ATOM | 816 817 818 819 | NZ N CA C | LYS L LEU L LEU L | 104 104 104 | 15.498 15.990 16.781 16.987 16.046 | 13.689 17.639 18.856 19.533 19.828 | 20.882 14.815 14.684 16.045 16.770 | 1.00 87.84 1.00 35.10 1.00 36.62 1.00 33.72 1.00 39.22 | L L L L | N C C |
| 65 | ATOM ATOM ATOM ATOM ATOM | 820 821 822 823 824 | | LEU L LEU L LEU L LEU L LEU L | 104 104 104 | 16.046 16.027 16.698 18.031 15.830 | 19.791 21.156 21.069 22.140 | 13.731 13.559 12.812 12.772 | 1.00 40.97 1.00 36.66 1.00 43.72 1.00 37.07 | L L L | 0000 |
| | | | | | | 776 | | | | | |

| | MOTA MOTA MOTA MOTA | 825 826 827 828 | N CA C O | GLU L 105 GLU L 105 GLU L 105 GLU L 105 | 5 | 18.238 18.596 19.421 20.169 | 19.751 20.461 21.719 21.804 | 16.437 17.664 17.371 16.404 | 1.00 41.16 1.00 40.54 1.00 37.89 1.00 40.95 | L L L | С И |
|----|--------------------------------------|--|------------------------------|--|----------------------------|--|--|--|--|------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM | 829 830 831 832 833 | CB CG CD OE1 OE2 | GLU L 10 | 5 | 19.387 20.901 21.554 21.525 22.080 | 19.507 19.663 19.582 20.570 18.519 | 18.564 18.407 19.768 20.491 20.101 | 1.00 42.35 1.00 73.68 1.00 84.81 1.00 80.17 1.00 87.53 | L L L L | C C C O O N |
| 10 | MOTA MOTA MOTA MOTA MOTA | 834 835 836 837 838 | N CA C O CB | ILE L 100 | 5 5 | 19.229 19.880 21.054 20.938 18.833 | 22.737 24.019 24.258 24.188 25.123 | 18.229 17.981 18.933 20.148 18.154 | 1.00 36.04 1.00 42.09 1.00 43.14 1.00 41.05 1.00 37.55 | r r r | N C C |
| 15 | ATOM ATOM ATOM ATOM ATOM | 839 840 841 842 843 | CG1 CG2 CD1 N CA | | 5 5 7 | 18.110 19.520 16.795 22.235 23.426 | 25.383 26.432 24.610 24.505 24.732 | 16.829 18.579 16.726 18.331 19.142 | 1.00 47.08 1.00 49.18 1.00 53.81 1.00 43.16 1.00 42.21 | r r r | С С И С |
| 20 | ATOM ATOM ATOM ATOM | 844 845 846 847 | C O CB CG | LYS L 10 LYS L 10 LYS L 10 LYS L 10 LYS L 10 | 7 . 7 7 | 23.359 23.424 24.645 24.960 26.185 | 26.065 27.140 24.716 23.313 23.302 | 19.892 19.311 18.219 17.696 16.778 | 1.00 45.78 1.00 52.84 1.00 43.56 1.00 41.44 1.00 36.40 | L L L L | 00000 |
| 25 | MOTA ATOM ATOM ATOM ATOM ATOM | 848 849 850 851 852 | CE NZ N CA | LYS L 10 LYS L 10 LYS L 10 LYS L 10 | 7 7 8 8 | 26.513 27.650 23.271 23.241 | 21.899 21.965 25.992 27.168 27.279 | 16.261 15.344 21.213 22.068 22.779 | 1.00 60.78 1.00 61.58 1.00 51.53 1.00 46.01 1.00 51.04 | L L L | C N C C |
| 30 | ATOM ATOM ATOM ATOM ATOM | 853 854 855 856 857 | C O CB CG CD | LYS L 10 LYS L 10 LYS L 10 LYS L 10 LYS L 10 | 8 8 8 | 24.585 25.443 22.125 22.058 21.059 | 26.395 27.015 28.136 27.871 | 22.653 23.106 24.099 25.178 | 1.00 52.80 1.00 40.77 1.00 40.59 1.00 24.84 | L L L | 0000 |
| 35 | MOTA MOTA MOTA MOTA | 858 859 860 861 862 | CE NZ N CA C | LYS L 10 LYS L 10 ALA L 10 ALA L 10 | 8 9 9 | 21.135 22.525 24.774 26.000 25.841 | 28.956 29.139 28.370 28.567 27.746 | 26.237 26.754 23.513 24.273 25.539 | 1.00 44.44 1.00 37.04 1.00 52.73 1.00 52.89 1.00 52.68 | r r r | N C C |
| 40 | ATOM ATOM ATOM ATOM ATOM | 863 864 865 866 867 | O CB N CA C | ALA L 10 ALA L 10 ASP L 11 ASP L 11 | 9 .0 .0 | 24.728 26.177 26.944 26.902 26.142 | 27.608 30.033 27.200 26.392 27.082 | 26.052 24.626 26.039 27.252 28.385 | 1.00 47.67 1.00 55.47 1.00 52.11 1.00 48.45 1.00 47.36 | L L L L | О С О |
| 45 | MOTA MOTA MOTA | 868 869 870 871 | O CB CG OD: | ASP L 11 ASP L 11 ASP L 11 L ASP L 11 | .0 .0 .0 .0 | 26.241 28.320 29.003 28.396 30.160 | 28.294 26.060 25.027 24.574 24.663 | 28.580 27.715 26.829 25.826 27.147 | 1.00 43.93 1.00 43.82 1.00 58.57 1.00 54.58 1.00 62.28 | L L L L | 0 0 0 0 |
| 50 | MOTA MOTA MOTA MOTA MOTA | 872 873 874 875 876 877 | N CA C O CB | 2 ASP L 11 ALA L 13 ALA L 13 ALA L 13 ALA L 13 ALA L 13 | .1 .1 .1 .1 | 25.368 24.592 24.644 24.586 23.148 | 26.294 26.797 25.726 24.530 27.052 | 29.120 30.246 31.315 31.005 29.832 | 1.00 44.56 1.00 39.67 1.00 44.68 1.00 49.08 1.00 31.81 | r r r | С С И |
| 55 | ATOM ATOM ATOM ATOM ATOM | 878 879 880 881 | N CA C O CB | ALA L 1: ALA L 1: ALA L 1: ALA L 1: ALA L 1: | .2 .2 .2 .2 | 24.773 24.825 23.429 22.647 25.758 | 26.152 25.227 25.074 26.029 25.749 | 32.569 33.694 34.249 34.276 34.772 | 1.00 46.60 1.00 39.75 1.00 41.14 1.00 43.49 1.00 36.82 | L L L L | С С С |
| 60 | MOTA MOTA MOTA MOTA MOTA | 882 883 884 885 886 | N CA C O | PRO L 1: PRO L 1: PRO L 1: PRO L 1: | L3 L3 L3 L3 | 23.090 21.778 21.460 22.357 | 23.862 | 34.696 35.265 36.542 37.263 | 1.00 38.43 1.00 39.80 1.00 37.82 1.00 39.66 | L L L L | и С С |
| 65 | MOTA ATOM ATOM ATOM ATOM ATOM | 887 888 889 890 891 892 | N CA C | PRO L 1 PRO L 1 THR L 1 | 13 13 14 14 14 | 21.868 23.329 23.973 20.168 19.667 19.180 18.103 | 21.868 22.689 24.487 25.151 23.966 | 35.833 34.749 36.793 37.983 38.801 | 1.00 35.81 1.00 40.04 1.00 35.18 1.00 38.10 1.00 40.59 | L L L L | C C N C C |
| | MOTA | 893 | J | ד רד ידודי | | | | | | | |

| | ATOM | 894 | СВ | THR L | | 18.476 | 26.033 | 37.650 | 1.00 40.4 | | L | С |
|----|--------------|------------|------------|----------------|------------|-----------------------|------------------|------------------|--------------------------|---|--------|--------|
| | ATOM ATOM | 895 896 | OG1 CG2 | THR L | 114 | 18.814 | 26.882 | 36.555 | 1.00 56.0 | | L | 0 |
| | ATOM | 897 | N CG2 | | 114 115 | 18.088 19.966 | 26.872 23.555 | 38.835 39.787 | 1.00 39.9 | | Ē | C |
| 5 | ATOM | 898 | ČA | VAL L | | 19.604 | 22.388 | 40.574 | 1.00 40.8 | | L L | N C |
| | ATOM | 899 | C | VAL L | 115 | 18.839 | 22.704 | 41.840 | 1.00 40.0 | | Ŀ | ď |
| | ATOM | 900 | 0 | | 115 | 19.175 | 23.638 | 42.557 | 1.00 49.0 | | L | ŏ |
| | ATOM | 901 | CB | | 115 | 20.855 | 21.587 | 40.936 | 1.00 34.5 | | L | C |
| 10 | MOTA MOTA | 902 903 | CG1 | | 115 | 20.461 | 20.220 | 41.428 | 1.00 34.9 | | L | C |
| 10 | ATOM | 904 | N | SER L | | 21.767 17.797 | 21.478 21.926 | 39.724 42.110 | 1.00 34.5 1.00 42.2 | | L | C |
| | ATOM | 905 | CA | SER L | | 16.997 | 22.124 | 43.314 | 1.00 42.2 | | L L | N C |
| | MOTA | 906 | С | SER L | | 16.432 | 20.781 | 43.768 | 1.00 44.2 | | Ŀ | C |
| | ATOM | 907 | 0 | | 116 | 15.787 | 20.071 | 42.994 | 1.00 43.6 | | L | ŏ |
| 15 | ATOM ATOM | 908 | CB | SER L | | 15.867 | 23.137 | 43.063 | 1.00 44.7 | _ | L | C |
| | ATOM | 909 910 | OG N | SER L ILE L | 116 | 14.936 16.690 | 22.668 20.445 | 42.114 | 1.00 40.3 | | Ŀ | 0 |
| | ATOM | 911 | CA | ILE L | | 16.259 | 19.178 | 45.030 45.611 | 1.00 45.4 1.00 43.5 | | L | N |
| | ATOM | 912 | C | ILE L | | 14.991 | 19.319 | 46.444 | 1.00 43.3 | | L L | C |
| 20 | MOTA | 913 | 0 | ILE L | | 14.690 | 20.395 | 46.934 | 1.00 49.2 | | L | ŏ |
| | ATOM | 914 | СВ | ILE L | | 17.390 | 18.586 | 46.475 | 1.00 41.5 | | L | Č |
| | ${f ATOM}$ | 915 916 | CG1 CG2 | | | 17.039 | 17.160 | 46.902 | 1.00 42.5 | | L | C |
| | ATOM | 917 | | ILE L ILE L | | 17.645 18.205 | 19.484 16.384 | 47.658 47.448 | 1.00 33.2 1.00 24.0 | | L | C |
| 25 | ATOM | 918 | N | PHE L | | 14.250 | 18.225 | 46.598 | 1.00 24.0 | | L L | C N |
| | ATOM | 919 | CA | PHE L | | 13.001 | 18.247 | 47.347 | 1.00 39.9 | | L | G |
| | ATOM | 920 | C | PHE L | | 12.783 | 17.035 | 48.247 | 1.00 42.6 | - | L | č |
| | ATOM ATOM | 921 | O | PHE L | | 12.931 | 15.895 | 47.812 | 1.00 40.7 | | L | 0 |
| 30 | ATOM | 922 923 | CB CG | PHE L PHE L | | 11.814 11.817 | 18.355 | 46.387 | 1.00 35.4 | | L | C |
| 00 | ATOM | 924 | | PHE L | | 12.716 | 19.600 19.753 | 45.553 44.514 | 1.00 34.5 1.00 18.8 | - | L L | C |
| | ATOM | 925 | CD2 | | 118 | 10.912 | 20.621 | 45.806 | 1.00 30.7 | | ь Г | C |
| | MOTA | 926 | CE1 | | 118 | 12.717 | 20.894 | 43.741 | 1.00 32.1 | | Ē | C |
| 05 | ATOM | 927 | CE2 | | | 10.909 | 21.771 | 45.031 | 1.00 31.2 | 2 | L | Č |
| 35 | ATOM ATOM | 928 929 | CZ | PHE L | | 11.815 | 21.905 | 43.995 | 1.00 25.1 | | L | С |
| | ATOM | 930 | N CA | PRO L PRO L | | 12.421 12.169 | 17.278 16.224 | 49.523 50.512 | 1.00 47.9 | | L | N |
| | ATOM | 931 | C | PRO L | | 10.819 | 15.591 | 50.312 | 1.00 47.9 1.00 48.2 | | L L | C C |
| | ATOM | 932 | 0 | PRO L | | 10.000 | 16.180 | 49.507 | 1.00 54.1 | | L | Ö |
| 40 | ATOM | 933 | CB | PRO L | | 12.151 | 16.985 | 51.840 | 1.00 48.8 | | L | Ċ |
| | ATOM | 934 | CG | PRO L | - | 12.940 | 18.236 | 51.547 | 1.00 44.7 | - | L | C |
| | ATOM ATOM | 935 936 | CD N | PRO L : | 119 120 | 12.467 | 18.597 | 50.180 | 1.00 43.8 | | L | C |
| | ATOM | 937 | CA | PRO L | | 10.570 9.312 | 14.385 13.665 | 50.738 50.524 | 1.00 45.7 1.00 42.2 | | L | N |
| 45 | MOTA | 938 | C | PRO L | - | 8.133 | 14.384 | 51.149 | 1.00 42.2 | | L L | C |
| | ATOM | 939 | 0 | | 120 | 8.243 | 14.972 | 52.224 | 1.00 41.7 | | L | ŏ |
| | ATOM | 940 | CB | PRO L : | | 9.552 | 12.322 | 51.206 | 1.00 42.9 | | L | C |
| | ATOM ATOM | 941 942 | CG CD | PRO L | | 11.046 | 12.173 | 51.177 | 1.00 53.9 | | L | C |
| 50 | ATOM | 943 | И | PRO L : | | 11.516 7.000 | 13.562 14.333 | 51.506 50.464 | 1.00 48.0 1.00 51.3 | | L | C |
| | ATOM | 944 | CA | SER L | | 5.783 | 14.941 | 50.970 | 1.00 52.6 | | L L | N C |
| | ATOM | 945 | С | SER L | 121 | 5.304 | 14.072 | 52.132 | 1.00 54.3 | | L | Č |
| | ATOM | 946 | 0 | SER L | | 5.426 | 12.842 | 52.102 | 1.00 56.7 | | L | ŏ |
| 55 | ATOM ATOM | 947 | CB | SER L | | 4.714 | 14.972 | 49.878 | 1.00 47.4 | | L | C |
| 55 | ATOM | 948 949 | OG N | SER L 3 | | $4.352 \\ 4.775$ | 13.655 14.711 | 49.491 | 1.00 54.1 | | L | 0 |
| | ATOM | 950 | CA | SER L | | $\frac{4.775}{4.270}$ | 13.971 | 53.168 54.317 | 1.00 60.00 1.00 59.80 | | L L | N |
| | ATOM | 951 | C | SER L | | 3.155 | 13.072 | 53.802 | 1.00 56.6 | | L L | C |
| | MOTA | 952 | 0 | SER L 3 | | 2.985 | 11.939 | 54.251 | 1.00 61.42 | | L | Ö |
| 60 | MOTA | 953 | CB | SER L 3 | | 3.710 | 14.938 | 55.351 | 1.00 64.43 | 3 | L | Č |
| | ATOM | 954 | OG | SER L 1 | | 2.595 | 15.630 | 54.816 | 1.00 74.50 | | L | 0 |
| | ATOM ATOM | 955 956 | N CA | GLU L 1 | | $2.407 \\ 1.298$ | 13.597 | 52.838 | 1.00 52.93 | | L | N |
| | ATOM | 957 | CA | GLU L 1 | | 1.298 1.745 | 12.884 11.552 | 52.225 51.657 | 1.00 54.30 | | L L | C |
| 65 | ATOM | 958 | Ö | GLU L 1 | | 1.092 | 10.532 | 51.858 | 1.00 57.02 | | L L | C O |
| | MOTA | 959 | CB | GLU L 1 | l.23 | 0.691 | 13.745 | 51.129 | 1.00 56.56 | | L | Č |
| | MOTA | 960 | CG | GLU L 1 | | 0.287 | 15.109 | 51.631 | 1.00 70.52 | 2 | L | С |
| | ATOM ATOM | 961 962 | CD OF1 | GLU L 1 | | -0.272 | 15.981 | 50.545 | 1.00 89.26 | | L | C |
| | WI OIL | 202 | OUT | GLU L 1 | LZJ | -1.246 | 15.550 | 49.890 | 1.00 82.90 |) | L | 0 |

| | Th .deser | | | | | | | | | |
|----|--------------|------------|---------|------------------------|----------------|----------------|------------------|--------------------------|--------|-----|
| | ATOM | 963 | OE2 | GLU L 123 | 0.266 | 17.095 | 50.351 | 1.00 95.75 | I | . 0 |
| | MOTA | 964 | N | GLN L 124 | 2.856 | 11.556 | 50.935 | 1.00 55.07 | Ī | |
| | MOTA | 965 | CA | GLN L 124 | 3.357 | 10.311 | 50.384 | 1.00 54.12 | I | |
| | ATOM | 966 | C | GLN L 124 | 3.868 | 9.459 | 51.532 | 1.00 52.45 | I | |
| 5 | ATOM | 967 | 0 | GLN L 124 | 3.770 | 8.229 | 51.505 | 1.00 49.04 | I | |
| | MOTA | 968 | CB | GLN L 124 | 4.490 | 10.568 | 49.401 | 1.00 55.78 | I | |
| | MOTA | 969 | CG | GLN L 124 | 5.223 | 9.297 | 49.028 | 1.00 56.57 | I | |
| | MOTA | 970 | CD | GLN L 124 | 6.372 | 9.546 | 48.103 | 1.00 50.07 | I | r c |
| | MOTA | 971 | | GLN L 124 | 6.949 | 10.636 | 48.087 | 1.00 46.99 | I | · 0 |
| 10 | ATOM | 972 | NE2 | GLN L 124 | 6.730 | 8.534 | 47.329 | 1.00 51.34 | I | N |
| | MOTA | 973 | M | LEU L 125 | 4.421 | 10.131 | 52.537 | 1.00 52.12 | I | L N |
| | ATOM | 974 | CA | LEU L 125 | 4.955 | 9.455 | 53.708 | 1.00 55.42 | I | |
| | MOTA | 975 | С | LEU L 125 | 3.856 | 8.732 | 54.463 | 1.00 62.18 | I | r C |
| | ATOM | 976 | 0 | LEU L 125 | 4.020 | 7.573 | 54.852 | 1.00 63.10 | I | |
| 15 | ATOM | 977 | CB | LEU L 125 | 5.655 | 10.456 | 54.626 | 1.00 51.50 | I | |
| | ATOM | 978 | CG | LEU L 125 | 7.041 | 10.877 | 54.130 | 1.00 58.49 | I | G C |
| | ATOM | 979 | | LEU L 125 | 7.614 | 11.993 | 54.997 | 1.00 55.80 | I | |
| | MOTA | 980 | | LEU L 125 | 7.955 | 9.657 | 54.132 | 1.00 41.53 | I | |
| | ATOM | 981 | N | THR L 126 | 2.728 | 9.405 | 54.666 | 1.00 67.91 | I | |
| 20 | ATOM | 982. | CA | THR L 126 | 1.625 | 8.772 | 55.374 | 1.00 74.12 | I | |
| | ATOM | 983 | Ğ | THR L 126 | 1.338 | 7.457 | 54.665 | 1.00 72.07 | I | |
| | MOTA | 984 | 0_ | THR L 126 | 0.825 | 6.519 | 55.259 | 1.00 74.16 | I | |
| | ATOM | 985 | CB | THR L 126 | 0.341 | 9.643 | 55.362 | 1.00 74.87 | I | |
| 05 | ATOM | 986 | | THR L 126 | -0.109 | 9.818 | 54.015 | 1.00 89.50 | I | |
| 25 | MOTA | 987 | CG2 | | 0.604 | 11.004 | 55.982 | 1.00 77.06 | Ī | |
| | ATOM | 988 | N | SER L 127 | 1.690 | 7.401 | 53.386 | 1.00 73.54 | I | |
| | ATOM | 989 | CA | SER L 127 | 1.476 | 6.210 | 52.574 | 1.00 74.09 | Ī | |
| | ATOM | 990 | C | SER L 127 | 2.543 | 5.136 | 52.794 | 1.00 71.41 | I | |
| 30 | ATOM | 991 | 0 | SER L 127 | 2.361 | 3.990 | 52.400 | 1.00 68.13 | ī | |
| 30 | ATOM | 992 | CB | SER L 127 | 1.434 | 6.597 | 51.093 | 1.00 75.35 | I | |
| | ATOM ATOM | 993 994 | OG | SER L 127 | 1.480 | 5.449 | 50.265 | 1.00 79.24 | I | |
| | ATOM | | N | GLY L 128 | 3.655 | 5.508 | 53.417 | 1.00 67.28 | Ī | - |
| | ATOM | 995 996 | CA | GLY L 128 | 4.709 | 4.542 | 53.670 | 1.00 63.17 | Ĩ | |
| 35 | ATOM | 997 | C | GLY L 128 GLY L 128 | 5.868 | 4.598 | 52.670 | 1.00 61.71 | I | |
| 33 | MOTA | 998 | O | GLY L 129 | 6.795 | 3.799 | 52.708 | 1.00 55.67 | I | |
| | ATOM | 999 | N CA | GLY L 129 | 5.776 6.789 | 5.630 5.742 | 51.815 | 1.00 60.01 | I | |
| | ATOM | 1000 | CA | GLY L 129 | 7.540 | 7.051 | 50.784 50.994 | 1.00 51.52 | I | |
| | ATOM | 1001 | Ö | GLY L 129 | 7.077 | 7.031 | 51.711 | 1.00 54.47 1.00 56.91 | I I | |
| 40 | MOTA | 1001 | N | ALA L 130 | 8.711 | 7.162 | 50.390 | 1.00 36.91 | I. | - |
| 40 | MOTA | 1003 | CA | ALA L 130 | 9.509 | 8.360 | 50.512 | 1.00 43.26 | L | |
| | ATOM | 1004 | C | ALA L 130 | 10.162 | 8.574 | 49.169 | 1.00 44.36 | L | |
| | ATOM | 1005 | ŏ | ALA L 130 | 10.851 | 7.697 | 48.658 | 1.00 44.31 | ī | |
| | ATOM | 1006 | ČВ | ALA L 130 | 10.563 | 8.188 | 51.586 | 1.00 51.51 | Ī | |
| 45 | ATOM | 1007 | N | SER L 131 | 9.915 | 9.733 | 48.581 | 1.00 44.50 | Ī | |
| | MOTA | 1008 | CA | SER L 131 | 10.498 | 10.057 | 47.297 | 1.00 40.37 | Ī | |
| | ATOM | 1009 | C | SER L 131 | 11.226 | 11.385 | 47.391 | 1.00 43.32 | Ī | _ |
| | ATOM | 1010 | 0 | SER L 131 | 10.664 | 12.402 | 47.807 | 1.00 48.95 | I | |
| | MOTA | 1011 | CB | SER L 131 | 9.419 | 10.114 | 46.214 | 1.00 38.70 | I | |
| 50 | MOTA | 1012 | OG | SER L 131 | 8.904 | 8.820 | 45.949 | 1.00 36.52 | L | |
| | ATOM | 1013 | N | VAL L 132 | 12.497 | 11.354 | 47.032 | 1.00 38.46 | L | |
| | MOTA | 1014 | CA | VAL L 132 | 13.311 | 12.543 | 47.049 | 1.00 34.22 | I | |
| | MOTA | 1015 | C | VAL L 132 | 13.461 | 12.881 | 45.579 | 1.00 39.02 | L | |
| | ATOM | 1016 | 0 | VAL L 132 | 13.935 | 12.066 | 44.797 | 1.00 42.97 | L | |
| 55 | MOTA | 1017 | СВ | VAL L 132 | 14.666 | 12.237 | 47.658 | 1.00 38.34 | I | |
| | MOTA | 1018 | CG1 | VAL L 132 | 15.373 | 13.520 | 48.062 | 1.00 35.88 | L | |
| | ATOM | 1019 | CG2 | VAL L 132 | 14.473 | 11.310 | 48.833 | 1.00 45.84 | L | |
| | MOTA | 1020 | N | VAL L 133 | 13.023 | 14.070 | 45.191 | 1.00 35.71 | L | |
| | MOTA | 1021 | CA | VAL L 133 | 13.118 | 14.457 | 43.799 | 1.00 35.51 | L | |
| 60 | ATOM | 1022 | C | VAL L 133 | 14.107 | 15.610 | 43.629 | 1.00 35.39 | L | |
| | MOTA | 1023 | 0 | VAL L 133 | 14.332 | 16.406 | 44.537 | 1.00 32.94 | L | |
| | MOTA | 1024 | CB | VAL L 133 | 11.716 | 14.809 | 43.225 | 1.00 23.82 | L | C |
| | ATOM | 1025 | | VAL L 133 | 11.857 | 15.359 | 41.830 | 1.00 27.79 | L | C |
| | ATOM | 1026 | | VAL L 133 | 10.822 | 13.581 | 43.226 | 1.00 38.91 | L | C |
| 65 | ATOM | 1027 | N | CYS L 134 | 14.724 | 15.667 | 42.460 | 1.00 38.30 | L | ı N |
| | ATOM | 1028 | CA | CYS L 134 | 15.705 | 16.689 | 42.189 | 1.00 41.29 | L | C |
| | MOTA | 1029 | C | CYS L 134 | 15.527 | 17.183 | 40.758 | 1.00 42.64 | L | C |
| | MOTA | 1030 | 0 | CYS L 134 | 15.368 | 16.388 | 39.829 | 1.00 43.51 | L | |
| | MOTA | 1031 | CB | CYS L 134 | 17.102 | 16.104 | 42.397 | 1.00 38.37 | L | C |
| | | | | | | | | | | |

| | MOTA MOTA | 1032 1033 | SG CYS L 134 N PHE L 135 | 18.395 15.519 | 17.355 18.502 | 42.642 40.590 | 1.00 65.37 1.00 42.83 1.00 38.04 | L L L | S N C |
|----|--------------|----------------|--------------------------------|------------------|------------------|------------------|--|--------------|-------------|
| | ATOM ATOM | 1034 1035 | CA PHE L 135 C PHE L 135 | 15.365 16.669 | 19.106 19.732 | 39.270 38.820 | 1.00 35.38 | L | č |
| 5 | ATOM | 1036 | O PHE L 135 | 17.424 | 20.277 | 39.616 | 1.00 38.80 | L | 0 |
| | ATOM | 1037 | CB PHE L 135 | 14.276 | 20.193 | 39.268 | 1.00 34.74 1.00 31.55 | L L | C |
| | ATOM | 1038 1039 | CG PHE L 135 CD1 PHE L 135 | 12.878 12.434 | 19.664 18.652 | 39.381 38.546 | 1.00 31.33 | Ľ. | Č |
| | ATOM ATOM | 1040 | CD2 PHE L 135 | 11.995 | 20.197 | 40.313 | 1.00 35.76 | L | C |
| 10 | ATOM | 1041 | CE1 PHE L 135 | 11.132 | 18.177 | 38.635 | 1.00 31.56 | L | C |
| | ATOM | 1042 | CE2 PHE L 135 | 10.690 | 19.726 18.711 | 40.408 39.563 | 1.00 27.93 1.00 30.83 | L L | C |
| | ATOM ATOM | $1043 \\ 1044$ | CZ PHE L 135 N LEU L 136 | 10.261 16.926 | 19.620 | 37.530 | 1.00 30.83 | L | N |
| | ATOM | 1044 | CA LEU L 136 | 18.103 | 20.184 | 36.907 | 1.00 31.58 | L | С |
| 15 | ATOM | 1046 | C LEU L 136 | 17.500 | 20.856 | 35.680 | 1.00 35.59 | Ŀ | C |
| | MOTA | 1047 | O LEU L 136 | 17.302 19.096 | 20.232 19.076 | 34.638 36.522 | 1.00 34.85 1.00 29.55 | L L | 0 |
| | ATOM ATOM | 1048 1049 | CB LEU L 136 CG LEU L 136 | 19.090 | 18.497 | 37.674 | 1.00 29.59 | L | Č |
| | ATOM | 1050 | CD1 LEU L 136 | 19.073 | 17.684 | 38.639 | 1.00 28.48 | \mathbf{L} | C |
| 20 | MOTA | 1051 | CD2 LEU L 136 | 21.050 | 17.626 | 37.114 | 1.00 33.08 | L | C |
| | MOTA | 1052 | N ASN L 137 | 17.183 16.554 | 22.134 22.851 | 35.815 34.723 | 1.00 35.66 1.00 35.50 | L L | N C |
| | MOTA MOTA | 1053 1054 | CA ASN L 137 C ASN L 137 | 17.380 | 23.822 | 33.891 | 1.00 30.57 | L | č |
| | ATOM | 1055 | O ASN L 137 | 18.269 | 24.511 | 34.382 | 1.00 31.68 | L | 0 |
| 25 | MOTA | 1056 | CB ASN L 137 | 15.321 | 23.563 | 35.260 | 1.00 39.89 | L | C |
| | ATOM | 1057 | CG ASN L 137 OD1 ASN L 137 | 14.334 13.480 | 22.601 23.001 | 35.894 36.681 | 1.00 35.35 1.00 34.80 | L L | Ö |
| | MOTA MOTA | 1058 1059 | ND2 ASN L 137 | 14.444 | 21.328 | 35.545 | 1.00 34.00 | Ŀ | N |
| | ATOM | 1060 | N ASN L 138 | 17.042 | 23.843 | 32.609 | 1.00 33.92 | L | N |
| 30 | MOTA | 1061 | CA ASN L 138 | 17.607 | 24.760 | 31.601 | 1.00 38.60 | L L | C |
| | MOTA | 1062 | C ASN L 138 O ASN L 138 | 19.153 19.819 | 24.748 25.738 | 31.533 31.809 | 1.00 41.40 1.00 48.42 | L L | Ö |
| | ATOM ATOM | 1063 1064 | O ASN L 138 CB ASN L 138 | | 26.173 | 31.913 | 1.00 36.37 | L | Č |
| | MOTA | 1065 | CG ASN L 138 | 15.615 | 26.150 | 32.093 | 1.00 34.07 | T. | C |
| 35 | MOTA | 1066 | OD1 ASN L 138 | | 26.138 | 33.205 | 1.00 52.45 1.00 45.49 | L L | N O |
| | MOTA | 1067 1068 | ND2 ASN L 138 N PHE L 139 | | 26.139 23.640 | 30.951 31.136 | 1.00 45.49 | L | N |
| | MOTA MOTA | 1069 | CA PHE L 139 | | 23.590 | 31.028 | 1.00 36.96 | $^{ m L}$ | C |
| | MOTA | 1070 | C PHE L 139 | 21.584 | 23.275 | 29.577 | 1.00 38.99 | L | C |
| 40 | ATOM | 1071 | O PHE L 139 | 20.727 | 22.950 | 28.756 31.992 | 1.00 31.96 1.00 34.96 | L L | 0 C |
| | ATOM ATOM | 1072 1073 | CB PHE L 139 CG PHE L 139 | | 22.529 21.174 | 31.814 | 1.00 34.30 | Ľ | Č |
| | ATOM | 1074 | CD1 PHE L 139 | | 20.373 | 30.746 | 1.00 28.85 | L | С |
| | ATOM | 1075 | CD2 PHE L 139 | | 20.726 | 32.677 | 1.00 30.19 | L | C |
| 45 | MOTA | 1076 | CE1 PHE L 139 CE2 PHE L 139 | | 19.152 19.504 | 30.533 32.476 | 1.00 26.26 1.00 29.02 | L L | C |
| | ATOM ATOM | 1077 1078 | CE2 PHE L 139 | | 18.712 | 31.401 | 1.00 29.39 | L | č |
| | MOTA | 1079 | N TYR L 140 | 22.865 | 23.389 | 29.257 | 1.00 44.67 | L | N |
| | MOTA | 1080 | CA TYR L 140 | 23.308 | 23.105 | 27.908 | 1.00 42.78 1.00 42.60 | L L | C |
| 50 | MOTA | 1081 1082 | C TYR L 140 O TYR L 140 | | 22.904 23.667 | 27.884 28.495 | 1.00 42.80 | Ľ. | Ö |
| | ATOM ATOM | 1082 | CB TYR L 140 | | 24.244 | 26.960 | 1.00 39.66 | L | С |
| | ATOM | 1084 | CG TYR L 140 | 23.239 | | 25.519 | 1.00 38.62 | L | C |
| | MOTA | 1085 | CD1 TYR L 140 | | 24.074 | 25.057 | 1.00 38.52 1.00 41.68 | L L | C |
| 55 | MOTA MOTA | 1086 1087 | CD2 TYR L 140 CE1 TYR L 140 | | 23.465 23.722 | 24.645 23.780 | 1.00 40.62 | L | Ğ |
| | MOTA | 1088 | CE2 TYR L 140 | | | 23.353 | 1.00 42.88 | L | С |
| | ATOM | 1089 | CZ TYR L 140 | 23.910 | 23.233 | 22.927 | 1.00 48.74 | L - | C |
| | MOTA | 1090 | OH TYR L 140 | | 22.864 21.883 | 21.651 27.148 | 1.00 52.93 1.00 43.92 | L L | Ŋ |
| 60 | MOTA MOTA | 1091 1092 | N PRO L 141 CA PRO L 141 | | | 26.365 | 1.00 46.65 | Ĺ | Ĉ |
| | ATOM | 1093 | C PRO L 141 | | | 27.185 | 1.00 49.80 | L | C |
| | MOTA | 1094 | O PRO L 143 | L 23.702 | 19.934 | 28.414 | 1.00 56.01 | L | 0 |
| | MOTA | 1095 | CB PRO L 143 | | | 25.414 26.256 | 1.00 45.66 1.00 41.16 | r F | G G |
| 65 | MOTA MOTA | 1096 1097 | CG PRO L 14: CD PRO L 14: | | | 26.236 | 1.00 41.10 | L | C |
| | ATOM | 1098 | N LYS L 14: | | | 26.494 | 1.00 47.16 | L | N |
| | MOTA | 1099 | CA LYS L 14: | 22.055 | 18.059 | 27.073 | 1.00 50.49 | L | C |
| | ATOM | 1100 | C LYS L 14: | 2 22.714 | 16.954 | 27.908 | 1.00 49.27 | L | С |

| | | | | | ••" | | | | | | |
|----|--------------|--------------|--------------|------------------------|-----|------------------|-----------------|------------------|--------------------------|---------|----------|
| | ATOM | 1101 | . 0 | LYS L 142 | | 22.068 | 16.216 | 28.642 | 1.00 52.27 | | _ |
| | MOTA | 1102 | | LYS L 142 | | 21.248 | 17.439 | | 1.00 32.27 | I | _ |
| | ATOM | 1103 | CG | LYS L 142 | | 22.141 | 16.757 | | 1.00 63.02 | I. I | _ |
| | ATOM | 1104 | CD | LYS L 142 | | 21.345 | 15.845 | | 1.00 58.35 | L | _ |
| 5 | MOTA | 1105 | CE | LYS L 142 | | 21.853 | 15.899 | | 1.00 73.15 | ī | _ |
| | MOTA | 1106 | NZ | LYS L 142 | | 23.168 | 15.269 | | 1.00 96.24 | Ī | _ |
| | MOTA | 1107 | N | ASP L 143 | | 24.044 | 16.825 | | 1.00 50.43 | L | |
| | ATOM | 1108 | | ASP L 143 | | 24.763 | 15.768 | | 1.00 55.24 | ī | |
| | ATOM | 1109 | С | ASP L 143 | | 25.076 | 16.163 | 29.902 | 1.00 53.06 | L | _ |
| 10 | MOTA | 1110 | | ASP L 143 | | 25.811 | 17.102 | 30.180 | 1.00 60.12 | L | _ |
| | MOTA | 1111 | СВ | ASP L 143 | | 26.070 | 15.493 | 27.705 | 1.00 58.45 | L | _ |
| | MOTA | 1112 | CG | ASP L 143 | | 25.787 | 14.678 | 26.452 | 1.00 74.50 | L | |
| | MOTA | 1113 | | L ASP L 143 | | 25.958 | 15.224 | 25.362 | 1.00 87.12 | L | |
| 15 | MOTA | 1114 | | 2 ASP L 143 | | 25.432 | 13.507 | 26.575 | 1.00 96.79 | L | 0 |
| 15 | ATOM ATOM | 1115 | N | ILE L 144 | | 24.460 | 15.425 | 30.845 | 1.00 49.84 | L | N |
| | ATOM | 1116 1117 | CA | ILE L 144 | | 24.740 | 15.678 | 32.255 | 1.00 43.94 | L | С |
| | MOTA | 1118 | C | ILE L 144 | | 24.481 | 14.437 | 33.110 | 1.00 44.67 | L | C |
| | ATOM | 1119 | CB | ILE L 144 ILE L 144 | | 23.746 | 13.529 | 32.743 | 1.00 46.34 | L | |
| 20 | ATOM | 1120 | CG1 | | | 23.852 | 16.828 | 32.730 | 1.00 47.26 | L | |
| | MOTA | 1121 | CG2 | | | 24.187 22.377 | 17.188 | 34.181 | 1.00 39.55 | L | |
| | ATOM | 1122 | | . ILE L 144 | | 23.503 | 16.390 | 32.685 | 1.00 27.85 | L | |
| | ATOM | 1123 | N | ASN L 145 | | 25.153 | 18.480 14.402 | 34.636 | 1.00 37.00 | L | _ |
| | ATOM | 1124 | ČA | ASN L 145 | | 24.977 | 13.263 | 34.274 35.167 | 1.00 47.86 | L | |
| 25 | ATOM | 1125 | C | ASN L 145 | | 24.543 | 13.703 | 36.565 | 1.00 56.19 | L | |
| | ATOM | 1126 | ō | ASN L 145 | | 24.971 | 14.722 | 37.097 | 1.00 48.41 1.00 51.90 | Ļ | _ |
| | ATOM | 1127 | CB | ASN L 145 | | 26.308 | 12.514 | 35.257 | 1.00 51.90 | ŗ | |
| | MOTA | 1128 | CG | ASN L 145 | | 26.692 | 11.994 | 33.896 | 1.00 79.58 | L | |
| | MOTA | 1129 | | ASN L 145 | | 25.875 | 11.463 | 33.148 | 1.00 74.98 | L | C |
| 30 | ATOM | 1130 | | ASN L 145 | | 27.992 | 12.137 | 33.582 | 1.00 74.98 | L L | |
| | ATOM | 1131 | N | VAL L 146 | | 23.627 | 12.907 | 37.144 | 1.00 47.14 | F. | |
| | MOTA | 1132 | CA | VAL L 146 | | 23.220 | 13.153 | 38.521 | 1.00 41.80 | L | N C |
| | ATOM | 1133 | С | VAL L 146 | | 23.646 | 12.000 | 39.432 | 1.00 41.27 | Ŀ | C |
| | MOTA | 1134 | 0 | VAL L 146 | | 23.665 | 10.840 | 39.043 | 1.00 41.13 | L | 0 |
| 35 | MOTA | 1135 | CB | VAL L 146 | | 21.700 | 13.305 | 38.550 | 1.00 38.57 | L | Č |
| | MOTA | 1136 | CG1 | VAL L 146 | | 21.222 | 13.420 | 39.996 | 1.00 48.70 | L | C |
| | ATOM | 1137 | CG2 | VAL L 146 | | 21.291 | 14.552 | 37.788 | 1.00 52.23 | L | č |
| | MOTA | 1138 | \mathbf{N} | LYS L 147 | | 24.019 | 12.322 | 40.657 | 1.00 39.29 | L | N |
| 40 | ATOM | 1139 | ca | LYS L 147 | | 24.434 | 11.308 | 41.580 | 1.00 43.68 | L | Ĉ |
| 40 | ATOM | 1140 | C | LYS L 147 | | 23.757 | 11.587 | 42.893 | 1.00 43.43 | L | Č |
| | ATOM | 1141 | 0 | LYS L 147 | | 23.829 | 12.680 | 43.439 | 1.00 47.08 | L | ŏ |
| | ATOM | 1142 | CB | LYS L 147 | | 25.952 | 11.402 | 41.744 | 1.00 43.41 | L | Ċ |
| | ATOM | 1143 | CG | LYS L 147 | | 26.521 | 10.238 | 42.559 | 1.00 49:00 | L | Ċ |
| 45 | ATOM | 1144 | CD | LYS L 147 | | 27.994 | 10.448 | 42.918 | 1.00 69.56 | L | Č |
| 45 | ATOM | 1145 | CE | LYS L 147 | | 28.883 | 10.597 | 41.679 | 1.00 79.19 | L | C |
| | MOTA | 1146 | NZ | LYS L 147 | | 29.949 | 11.561 | 41.950 | 1.00 85.36 | L | N |
| | ATOM | 1147 | N | TRP L 148 | | 23.051 | 10.591 | 43.410 | 1.00 49.19 | L | N |
| | ATOM ATOM | 1148 | CA | TRP L 148 | | 22.371 | 10.756 | 44.682 | 1.00 45.19 | L | C |
| 50 | ATOM | 1149 1150 | C | TRP L 148 | | 23.305 | 10.250 | 45.751 | 1.00 45.91 | Ŀ | C |
| 00 | ATOM | 1151 | O CB | TRP L 148 | | 24.076 | 9.322 | 45.529 | 1.00 43.97 | L | 0 |
| | ATOM | 1152 | CG | TRP L 148 TRP L 148 | | 21.065 | 9.964 | 44.727 | 1.00 39.66 | ${f L}$ | C |
| | ATOM | 1153 | | TRP L 148 | | 19.940 19.564 | 10.601 | 43.968 | 1.00 42.61 | L | С |
| | ATOM | 1154 | | TRP L 148 | | 19.029 | 10.346 | 42.677 | 1.00 33.06 | Ļ | С |
| 55 | ATOM | 1155 | NE1 | TRP L 148 | | 18.469 | 11.586 | 44.464 | 1.00 42.82 | L | C |
| | MOTA | 1156 | CE2 | TRP L 148 | | 18.121 | 11.107 11.879 | 42.344 | 1.00 30.84 | Ŀ | N |
| | MOTA | 1157 | CE3 | TRP L 148 | | 18.887 | 12.247 | 43.422 | 1.00 35.66 | L | C |
| | ATOM | 1158 | CZ2 | TRP L 148 | | 17.086 | 12.807 | 45.687 | 1.00 32.84 | L | C |
| | MOTA | 1159 | CZ3 | TRP L 148 | | 17.858 | 13.162 | 43.570 | 1.00 29.88 | L | C |
| 60 | ATOM | 1160 | | TRP L 148 | | 16.971 | 13.434 | 45.831 44.778 | 1.00 40.22 1.00 26.01 | L | C |
| | ATOM | 1161 | N | LYS L 149 | | 23.241 | 10.883 | 46.911 | | Ŀ | C |
| | ATOM | 1162 | CA | LYS L 149 | | 24.072 | 10.504 | 48.036 | 1.00 47.40 1.00 41.22 | L | И |
| | ATOM | 1163 | C | LYS L 149 | | 23.260 | 10.572 | 49.313 | | L | C |
| | MOTA | 1164 | ŏ | LYS L 149 | | 22.582 | 11.560 | 49.554 | 1.00 39.97 1.00 49.04 | L | C |
| 65 | ATOM | 1165 | СВ | LYS L 149 | | 25.267 | 11.454 | 48.162 | 1.00 49.04 | L L | 0 |
| | ATOM | 1166 | CG | LYS L 149 | | 26.501 | 11.060 | 47.373 | 1.00 35.13 | L | C |
| | MOTA | 1167 | CD | LYS L 149 | | 27.679 | 11.917 | 47.817 | 1.00 45.37 | Ľ | C |
| | MOTA | 1168 | CE | LYS L 149 | | 28.982 | 11.466 | 47.181 | 1.00 70.51 | L | C |
| | ATOM | 1169 | NZ | LYS L 149 | | 30.156 | 12.182 | 47.759 | 1.00 67.81 | L | N |
| | | | | | | | | | | _ | * |

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| | р чен ч | . , | | | | | | | | |
|------|--------------|--------------|-----------|----------------|------------------|-----------------------|------------------|--------------------------|--------------|--------|
| | ATOM | 1170 | N ILE L | 150 | 23.309 | 9.524 | 50.122 | 1.00 38.16 | L | N |
| | ATOM | 1171 | CA ILE L | | 22.606 | 9.544 | 51.396 | 1.00 38.62 | L | C |
| | MOTA | 1172 | C ILE I | | 23.624 | 9.285 | 52.498 | 1.00 39.38 | ŗ | C |
| | ATOM | 1173 | O ILE L | | 24.240 | 8.227 | 52.546 | 1.00 42.34 | L | 0 |
| 5 | MOTA | 1174 | CB ILE I | | 21.501 | 8.485 | 51.476 | 1.00 35.52 | L | C |
| | ATOM | 1175 | CG1 ILE I | | 20.483 | 8.700 | 50.351 | 1.00 34.00 | L | C |
| | ATOM | 1176 | CG2 ILE I | | 20.834 | 8.565 | 52.845 | 1.00 30.49 | L | C |
| | ATOM | 1177 | CD1 ILE I | | 19.319 | 7.730 | 50.350 | 1.00 21.56 | L | C |
| | MOTA | 1178 | N ASP I | | 23.799 | 10.263 | 53.379 | 1.00 42.16 | L | N |
| 10 | ATOM | 1179 | CA ASP I | | 24.763 | 10.162 | 54.468 | 1.00 43.08 1.00 47.39 | · <u>L</u> | C |
| | MOTA | 1180 | C ASP I | | 26.175 | 9.985 | 53.920 | 1.00 47.39 | L L | 0 |
| | ATOM | 1181 | O ASP I | | 26.964 | 9.180 | 54.422 | 1.00 33.21 | L L | C |
| | ATOM | 1182 | CB ASP I | | 24.408 23.255 | 9.001 9.328 | 55.395 56.307 | 1.00 38.76 | L | C |
| 4- | MOTA | 1183 1184 | CG ASP I | | 22.800 | 10.490 | 56.289 | 1.00 53.05 | L | ŏ |
| 15 . | ATOM ATOM | 1185 | ODI ASF I | | 22.806 | 8.434 | 57.048 | 1.00 49.41 | L | ŏ |
| | ATOM | 1186 | N GLY I | | 26.477 | 10.744 | 52.873 | 1.00 48.87 | L | N |
| | ATOM | 1187 | CA GLY I | | 27.819 | 10.665 | 52.287 | 1.00 46.37 | L | C |
| | ATOM | 1188 | C GLY I | | 27.938 | 9.582 | 51.203 | 1.00 49.77 | L | C |
| 20 | MOTA | 1189 | O GLY I | | 28.783 | 9.629 | 50.322 | 1.00 58.18 | L | 0 |
| | ATOM | 1190 | N SER I | | 27.077 | 8.554 | 51.312 | 1.00 48.01 | L | N |
| | MOTA | 1191 | CA SER I | 153 | 27.163 | 7.440 | 50.371 | 1.00 52.83 | L | C |
| | ATOM | 1192 | C SER I | 153 | 26.357 | 7.694 | 49.095 | 1.00 45.68 | L | С |
| | ATOM | 1193 | O SER I | 153 | 25.294 | 8.299 | 49.106 | 1.00 49.11 | L | 0 |
| 25 | ATOM | 1194 | CB SER I | | 26.634 | 6.189 | 51.082 | 1.00 54.79 | L | C |
| | MOTA | 1195 | OG SER I | | 27.612 | 5.715 | 52.009 | 1.00 69.58 | ŗ | 0 |
| | MOTA | 1196 | N GLU I | | 26.929 | 7.245 | 47.963 | 1.00 43.38 | L | N |
| | ATOM | 1197 | CA GLU I | | 26.197 | 7.333 | 46.703 | 1.00 50.29 | Ŀ | C |
| | ATOM | 1198 | C GLU I | | 25.117 | 6.253 | 46.615 | 1.00 49.87 1.00 56.57 | L L | C |
| 30 | ATOM | 1199 | O GLU I | | 25.273 27.194 | 5.136 7.167 | 47.088 45.553 | 1.00 36.57 | L | č |
| | MOTA | 1200 1201 | CB GLU I | | 26.582 | 6.459 | 44.340 | 1.00 43.07 | L | Č |
| | ATOM | 1201 | CD GLU I | | 27.464 | 6.677 | 43.126 | 1.00 72.03 | L | č |
| | MOTA MOTA | 1202 | OE1 GLU I | | 28.674 | 6.584 | 43.252 | 1.00 56.01 | Ĺ | Õ |
| 35 | ATOM | 1204 | OE2 GLU I | | 26.928 | 6.957 | 42.059 | 1.00 70.34 | L | ō |
| 55 | ATOM | 1205 | N ARG I | | 23.977 | 6.589 | 46.019 | 1.00 49.27 | L | N |
| | MOTA | 1206 | CA ARG I | | 22.910 | 5.615 | 45.804 | 1.00 47.42 | L | C |
| | ATOM | 1207 | C ARG I | | 22.739 | 5.463 | 44.293 | 1.00 48.15 | L | C |
| | ATOM | 1208 | O ARG I | | 22.790 | 6.446 | 43.554 | 1.00 49.72 | L | 0 |
| 40 | MOTA | 1209 | CB ARG I | i 155 | 21.584 | 6.075 | 46.418 | 1.00 45.78 | L | С |
| | MOTA | 1210 | CG ARG I | 155 | 21.489 | 5.965 | 47.938 | 1.00 46.29 | L | С |
| | MOTA | 1211 | CD ARG I | | 21.711 | 4.544 | 48.452 | 1.00 44.74 | L | C |
| | MOTA | 1212 | NE ARGI | | 21.593 | 4.481 | 49.908 | 1.00 46.03 | L | N |
| | MOTA | 1213 | CZ ARG I | | 20.450 | 4.313 | 50.565 | 1.00 47.68 | L | C |
| 45 | MOTA | 1214 | NH1 ARG I | | 19.314 | 4.173 | 49.902 | 1.00 57.00 | L | N |
| | MOTA | 1215 | NH2 ARG I | | 20.434 | 4.323 | 51.888 | 1.00 44.35 1.00 47.00 | L L | N N |
| | ATOM | 1216 | N GLN I | | 22.559 | 4.230 | 43.836 | 1.00 47.00 | r L | G |
| | MOTA | 1217 1218 | CA GLN I | | 22.375 21.002 | 3.956 3.359 | 42.416 42.205 | 1.00 48.51 | L | Č |
| 50 | MOTA MOTA | 1218 | O GLN | | 20.343 | 3.585 | 41.197 | 1.00 47.82 | L L | ŏ |
| 30 | ATOM | 1220 | | i 156 | 23.392 | 2.933 | 41.914 | 1.00 57.57 | L | Č |
| | MOTA | 1221 | | 156 | 24.813 | 3.404 | 41.730 | 1.00 69.42 | L | C |
| | MOTA | 1222 | | 156 | 25.459 | 2.736 | 40.522 | 1.00 87.97 | L | С |
| | ATOM | 1223 | OE1 GLN | | 25.401 | 1.514 | 40.364 | 1.00 94.85 | L | 0 |
| 55 | ATOM | 1224 | NE2 GLN | | 26.072 | 3.541 | 39.658 | 1.00 96.03 | L | N |
| | MOTA | 1225 | | ւ 157 | 20.584 | 2.583 | 43.188 | 1.00 50.75 | L | N |
| | MOTA | 1226 | | ւ 157 | 19.323 | 1.881 | 43.134 | 1.00 56.06 | L | C |
| | MOTA | 1227 | | L 157 | 18.104 | 2.729 | 43.475 | 1.00 51.01 | \mathbf{L} | C |
| | MOTA | 1228 | | և 157 | 18.185 | 3.662 | 44.263 | 1.00 54.53 | Ŀ | 0 |
| 60 | ATOM | 1229 | | L 157 | 19.434 | 0.668 | 44.060 | 1.00 63.75 | L | C |
| | MOTA | 1230 | | L 157 | 20.754 | -0.097 | 43.856 | 1.00 77.57 | L | C |
| | ATOM | 1231 | OD1 ASN | | 20.935 | -0.797 | 42.852 | 1.00 83.50 | L | O N |
| | MOTA | 1232 | ND2 ASN | | 21.689 | 0.060 | 44.800 42.852 | 1.00 79.77 1.00 46.82 | L L | N |
| C.E. | ATOM | 1233 | | L 158 | 16.978 15.743 | 2.402 3.113 | 42.852 | 1.00 46.62 | L L | C |
| 65 | MOTA MOTA | 1234 1235 | | ն 158 ն 158 | 15.631 | $\frac{3.113}{4.514}$ | 42.556 | 1.00 33.11 | L | Č |
| | ATOM | 1236 | | ь 158 ь 158 | 14.882 | 5.328 | 43.086 | 1.00 37.66 | L | ŏ |
| | ATOM | 1237 | | ь 159 | 16.364 | 4.818 | 41.496 | 1.00 33.40 | L | N |
| | MOTA | 1238 | | L 159 | 16.278 | 6.143 | 40.921 | 1.00 37.20 | L | C |
| | | | | | | | | | | |

| | ь | | | 8 ** | | | | | | |
|-----------|-----------------|------|-------------|-------|--------|--------|--------|------------|--------------|-----|
| | ATOM | 1239 | C VAL L 1 | 59 | 15.794 | 6.096 | 39.489 | 1.00 39.79 | L | С |
| | _ | | | .59 | 16.196 | 5.238 | 38.717 | 1.00 50.88 | L | 0 |
| | ATOM | 1240 | | | | | | 1.00 37.60 | ī. | č |
| | MOTA | 1241 | CB VAL L 1 | | 17.631 | 6.855 | 40.954 | | | Č |
| | ATOM | 1242 | CG1 VAL L 1 | | 18.728 | 5.839 | 41.060 | 1.00 41.29 | Ŀ | |
| 5 | ATOM | 1243 | CG2 VAL L 1 | .59 | 17.804 | 7.709 | 39.689 | 1.00 35.05 | ${f L}$ | С |
| | MOTA | 1244 | N LEU L 1 | .60 | 14.903 | 7.012 | 39.142 | 1.00 40.63 | L | N |
| | ATOM | 1245 | | .60 | 14.381 | 7.088 | 37.792 | 1.00 40.01 | L | С |
| | MOTA | 1246 | C LEU L 1 | | 14.539 | 8.525 | 37.298 | 1.00 35.48 | L | C |
| | MOTA | 1247 | O LEU L 1 | | 14.189 | 9.473 | 37.996 | 1.00 35.80 | L | 0 |
| 40 | | | | | 12.920 | 6.621 | 37.755 | 1.00 41.10 | L | č |
| 10 | ATOM | 1248 | CB LEU L 1 | | | 5.138 | 38.108 | 1.00 47.84 | Ľ | Č |
| | ATOM | 1249 | | .60 | 12.712 | | | | | |
| | MOTA | 1250 | CD1 LEU L 1 | .60 | 11.223 | 4.831 | 38.132 | 1.00 64.80 | Ţ | C |
| | MOTA | 1251 | CD2 LEU L 1 | | 13.380 | 4.229 | 37.103 | 1.00 43.08 | L | C |
| | MOTA | 1252 | N ASN L 1 | .61 | 15.110 | 8.661 | 36.104 | 1.00 33.90 | L | N |
| 15 | MOTA | 1253 | CA ASN L 1 | .61 | 15.383 | 9.949 | 35.479 | 1.00 32.64 | ${f L}$ | C |
| | ATOM | 1254 | | .61 | 14.524 | 10.192 | 34.260 | 1.00 33.50 | Ŀ | С |
| | ATOM | 1255 | | .61 | 14.149 | 9.265 | 33.559 | 1.00 38.43 | L | 0 |
| | ATOM | 1256 | | 61 | 16.828 | 10.007 | 35.003 | 1.00 38.36 | L | С |
| | | 1257 | CG ASN L 1 | | 17.823 | 9.762 | 36.101 | 1.00 37.26 | L | C |
| | ATOM | | | | 17.839 | 10.463 | 37.111 | 1.00 40.06 | L | ŏ ¹ |
| 20 | ATOM | 1258 | OD1 ASN L 1 | | | | | 1.00 32.15 | L | И |
| | ATOM | 1259 | ND2 ASN L 1 | | 18.678 | 8.769 | 35.902 | 1.00 32.13 | L | N |
| | MOTA | 1260 | N SER L 1 | | 14.249 | 11.452 | 33.976 | | | |
| | ATOM | 1261 | CA SER L 1 | | 13.462 | 11.777 | 32.800 | 1.00 26.43 | L | C |
| | ATOM | 1262 | C SER L 1 | L62 | 14.027 | 13.040 | 32.153 | 1.00 28.89 | Ŀ | C |
| 25 | MOTA | 1263 | O SER L 1 | L62 | 14.447 | 13.956 | 32.845 | 1.00 33.59 | L | 0 |
| | ATOM | 1264 | CB SER L 1 | L62 | 12.006 | 11.972 | 33.194 | 1.00 22.50 | \mathbf{L} | С |
| | ATOM | 1265 | OG SER L 1 | L62 | 11.191 | 11.991 | 32.046 | 1.00 37.37 | L | 0 |
| | ATOM | 1266 | N TRP L 1 | | 14.054 | 13.088 | 30.829 | 1.00 33.44 | L | N |
| | ATOM | 1267 | CA TRP L 1 | | 14.586 | 14.262 | 30.131 | 1.00 28.63 | L | C |
| 30 | ATOM | 1268 | C TRP L 1 | | 13.556 | 14.875 | 29.206 | 1.00 27.81 | L | С |
| 30 | | | O TRP L 1 | | 12.871 | 14.167 | 28.468 | 1.00 33.25 | L | Ö |
| | ATOM | 1269 | | | 15.817 | 13.888 | 29.293 | 1.00 28.11 | Ē | č |
| | ATOM | 1270 | | | | 13.331 | 30.084 | 1.00 30.72 | L | č |
| | ATOM | 1271 | CG TRP L 1 | | 16.950 | | | | | Ċ |
| | MOTA | 1272 | | 163 | 18.060 | 13.999 | 30.514 | 1.00 34.81 | L | |
| 35 | MOTA | 1273 | | 163 | 17.093 | 11.981 | 30.534 | 1.00 37.12 | Ŀ | C |
| | MOTA | 1274 | NE1 TRP L 1 | | 18.886 | 13.146 | 31.201 | 1.00 31.24 | L | N |
| | ATOM | 1275 | CE2 TRP L 1 | 163 | 18.317 | 11.899 | 31.227 | 1.00 36.59 | L | C |
| | ATOM | 1276 | CE3 TRP L 1 | 163 | 16.304 | 10.829 | 30.419 | 1.00 42.13 | L | С |
| | ATOM | 1277 | CZ2 TRP L 3 | 163 | 18.774 | 10.712 | 31.801 | 1.0044.40 | L | С |
| 40 | ATOM | 1278 | | 163 | 16.761 | 9.644 | 30.996 | 1.00 49.83 | L | C |
| -10 | ATOM | 1279 | CH2 TRP L | | 17.983 | 9.598 | 31.675 | 1.00 29.31 | L | C |
| | MOTA | 1280 | N THR L | | 13.463 | 16.199 | 29.235 | 1.00 27.83 | L | N |
| | | 1281 | CA THR L | | 12.531 | 16.916 | 28.377 | 1.00 29.47 | L | C |
| | MOTA | | | | 13.180 | 17.119 | 27.013 | 1.00 27.57 | Ī. | č |
| 45 | MOTA | 1282 | C THR L | | | 16.911 | 26.867 | 1.00 32.97 | L | ŏ |
| 45 | MOTA | 1283 | O THR L | | 14.379 | | | 1.00 32.57 | L | č |
| | ATOM | 1284 | CB THR L | | 12.215 | 18.292 | 28.955 | | | Ö |
| | \mathbf{MOTA} | 1285 | OG1 THR L | | 13.429 | 19.023 | 29.111 | 1.00 25.23 | L | - |
| | MOTA | 1286 | CG2 THR L | | 11.549 | 18.165 | 30.299 | 1.00 33.20 | Ŀ | C |
| | MOTA | 1287 | N ASP L | 165 | 12.393 | 17.499 | 26.009 | 1.00 32.30 | L | N |
| 50 | MOTA | 1288 | CA ASP L | 165 | 12.966 | 17.780 | 24.690 | 1.00 37.75 | \mathbf{L} | C |
| | MOTA | 1289 | C ASP L : | 165 | 13.614 | 19.155 | 24.807 | 1.00 34.76 | L | C |
| | MOTA | 1290 | O ASP L | 165 | 13.493 | 19.815 | 25.832 | 1.00 41.05 | L | 0 |
| | ATOM | 1291 | CB ASP L | | 11.890 | 17.835 | 23.597 | 1.00 44.29 | L | C |
| | ATOM | 1292 | CG ASP L | | 11.479 | 16.464 | 23.105 | 1.00 45.32 | L | C |
| EE | | | OD1 ASP L | | 10.645 | 15.818 | 23.769 | 1.00 54.61 | L | Ō |
| 55 | MOTA | 1293 | | | 11.998 | 16.033 | 22.052 | 1.00 65.66 | L | ŏ |
| | MOTA | 1294 | OD2 ASP L | | | | 23.772 | 1.00 34.89 | L | Ŋ |
| | MOTA | 1295 | N GLN L | | 14.294 | 19.615 | | | L | C |
| | MOTA | 1296 | CA GLN L | | 14.921 | 20.923 | 23.884 | 1.00 33.11 | | |
| | MOTA | 1297 | C GLN L | | 13.882 | 22.031 | 23.890 | 1.00 34.33 | L | C |
| 60 | MOTA | 1298 | O GLN L | | 12.917 | 22.001 | 23.126 | 1.00 40.73 | L | 0 |
| | ATOM | 1299 | CB GLN L | 166 | 15.927 | 21.130 | 22.754 | 1.00 32.34 | L | C |
| | MOTA | 1300 | CG GLN L | | 16.566 | 22.492 | 22.716 | 1.00 25.94 | ${f L}$ | C |
| | ATOM | 1301 | CD GLN L | | 17.735 | 22.524 | 21.767 | 1.00 24.29 | L | С |
| | ATOM | 1302 | OE1 GLN L | | 17.691 | 21.915 | 20.703 | 1.00 29.03 | L | 0 |
| 65 | ATOM | 1303 | NE2 GLN L | | 18.789 | 23.234 | 22.141 | 1.00 39.54 | L | N |
| 50 | ATOM | 1304 | N ASP L | | 14.084 | 23.000 | 24.775 | 1.00 36.26 | Ŀ | N |
| | | 1304 | CA ASP L | | 13.244 | 24.183 | 24.911 | 1.00 37.77 | Ē | Ĉ |
| | MOTA | | | | 13.133 | 24.919 | 23.578 | 1.00 38.98 | Ĺ | č |
| | ATOM | 1306 | | | | | 22.826 | 1.00 45.84 | , L | Ö |
| | MOTA | 1307 | O ASP L | T 0 \ | 14.089 | 25.044 | 22.020 | T.00 49.04 | ш | 0 |

| | ATOM | 1308 | СВ | ASP L | 167 | 13.869 | 25.102 | 25.965 | 1.00 39.01 | L | C |
|----|----------|------|-------------|-------|-------|--------|--------|--------|--------------------------|-------------|---|
| | ATOM | 1309 | CG | ASP L | | 12.825 | 26.104 | 26.438 | 1.00 50.62 | L | C |
| | ATOM | 1310 | | ASP L | | 11.843 | 25.665 | 27.041 | 1.00 61.30 | L L | |
| | - | 1311 | | ASP L | | | 27.301 | 26.214 | 1.00 65.60 | | 0 |
| _ | MOTA | | | | | 13.003 | | | | r L | 0 |
| 5 | ATOM | 1312 | N | SER L | | 11.907 | 25.373 | 23.265 | 1.00 39.91 | r P | N |
| | ATOM | 1313 | CA | SER L | | 11.711 | 26.041 | 21.985 | 1.00 36.41 | Ŀ | C |
| | ATOM | 1314 | C | SER L | | 12.002 | 27.542 | 22.067 | 1.00 36.74 | Ŀ | C |
| | ATOM | 1315 | 0_ | SER L | | 11.965 | 28.267 | 21.082 | 1.00 42.82 | L | 0 |
| | MOTA | 1316 | CB | SER L | | 10.268 | 25.802 | 21.535 | 1.00 34.55 | L | C |
| 10 | MOTA | 1317 | OG | SER L | | 10.172 | 24.514 | 20.922 | 1.00 38.70 | L | 0 |
| | MOTA | 1318 | N | LYS L | | 12.279 | 28.009 | 23.301 | 1.00 41.00 | L | N |
| | MOTA | 1319 | $^{\rm CA}$ | LYS L | | 12.476 | 29.440 | 23.491 | 1.00 40.71 | L | C |
| | MOTA | 1320 | С | LYS L | | 13.938 | 29.810 | 23.746 | 1.00 44.31 | L | C |
| | MOTA | 1321 | 0 | LYS L | 169 | 14.524 | 30.641 | 23.065 | 1.00 47.38 | L | 0 |
| 15 | MOTA | 1322 | $^{\rm CB}$ | LYS L | 169 | 11.596 | 29.896 | 24.654 | 1.00 50.40 | L | C |
| | MOTA | 1323 | CG | LYS L | 169 | 10.226 | 30.371 | 24.164 | 1.00 64.25 | L | C |
| | MOTA | 1324 | CD | LYS L | 169 | 9.232 | 30.585 | 25.307 | 1.00 92.37 | L | C |
| | MOTA | 1325 | CE | LYS L | 169 | 7.980 | 31.351 | 24.858 | 1.00 99.86 | L | C |
| | MOTA | 1326 | NZ | LYS L | 169 | 7.425 | 32.101 | 25.987 | 1.00 94.60 | L | N |
| 20 | ATOM | 1327 | N | ASP L | 170 | 14.514 | 29.200 | 24.799 | 1.00 45.97 | L | N |
| | ATOM | 1328 | CA | ASP L | | 15.922 | 29.466 | 25.091 | 1.00 46.90 | L | C |
| | ATOM | 1329 | C | ASP L | | 16.813 | 28.255 | 24.790 | 1.00 43.28 | L | C |
| | MOTA | 1330 | Ō | ASP L | | 17.967 | 28.170 | 25.193 | 1.00 47.78 | L | Õ |
| | ATOM | 1331 | ĊВ | ASP L | | 16.053 | 29.878 | 26.560 | 1.00 48.00 | L | Č |
| 25 | ATOM | 1332 | CG | ASP L | | 15.574 | 28.743 | 27.455 | 1.00 48.03 | L | č |
| | ATOM | 1333 | | ASP L | | 15.499 | 27.620 | 26.962 | 1.00 51.45 | L | ō |
| | ATOM | 1334 | | ASP L | | 15.296 | 28.988 | 28.627 | 1.00 84.97 | L | ŏ |
| | ATOM | 1335 | N | SER L | | 16.209 | 27.271 | 24.096 | 1.00 46.86 | Ŀ | N |
| | MOTA | 1336 | CA | SER L | | 16.983 | 26.133 | 23.607 | 1.00 48.35 | L | Č |
| 30 | ATOM | 1337 | C | SER L | | 17.845 | 25.485 | 24.692 | 1.00 48.37 | L L | Č |
| 50 | ATOM | 1338 | Õ | SER L | | 19.057 | 25.351 | 24.563 | 1.00 55.99 | L | Õ |
| | ATOM | 1339 | СВ | SER L | | 17.872 | 26.628 | 22.467 | 1.00 45.20 | L | C |
| | ATOM | 1340 | OG | SER L | | 17.053 | 26.974 | 21.348 | 1.00 43.20 | L | 0 |
| | | | | THR L | | 17.189 | 25.100 | 25.803 | | L | |
| 25 | MOTA | 1341 | N | THR L | | | | 26.856 | 1.00 51.34 1.00 44.78 | | N |
| 35 | MOTA | 1342 | CA | | | 17.921 | 24.407 | | | L | C |
| | ATOM | 1343 | C | THR L | | 17.399 | 22.982 | 27.059 | 1.00 42.17 | L | C |
| | MOTA | 1344 | O | THR L | | 16.466 | 22.535 | 26.405 | 1.00 45.97 | ŗ | 0 |
| | ATOM | 1345 | CB | THR L | | 17.783 | 25.207 | 28.152 | 1.00 37.85 | L | C |
| 40 | ATOM | 1346 | OG1 | | | 16.404 | 25.512 | 28.370 | 1.00 57.23 | \tilde{r} | 0 |
| 40 | MOTA | 1347 | CG2 | | | 18.577 | 26.517 | 28.050 | 1.00 33.68 | L | C |
| | ATOM | 1348 | N | TYR L | | 17.892 | 22.288 | 28.069 | 1.00 44.08 | Ŀ | N |
| | MOTA | 1349 | CA | TYR L | | 17.364 | 20.993 | 28.442 | 1.00 40.50 | L | C |
| | MOTA | 1350 | C | TYR L | | 17.228 | 20.919 | 29.947 | 1.00 40.14 | L | C |
| | MOTA | 1351 | 0 | TYR L | | 18.070 | 21.432 | 30.679 | 1.00 40.88 | L | 0 |
| 45 | ATOM | 1352 | CB | TYR L | | 18.299 | 19.877 | 28.014 | 1.00 32.40 | L | C |
| | MOTA | 1353 | CG | TYR L | | 18.551 | 19.773 | 26.544 | 1.00 38.44 | L | C |
| | ATOM | 1354 | CD1 | | | 19.528 | 20.542 | 25.931 | 1.00 23.34 | L | C |
| | MOTA | 1355 | CD2 | | 173 | 17.886 | 18.818 | 25.781 | 1.00 30.45 | L | C |
| | ATOM | 1356 | CE1 | | 173 | 19.847 | 20.347 | 24.605 | 1.00 23.64 | L | C |
| 50 | MOTA | 1357 | CE2 | | | 18.194 | 18.623 | 24.468 | 1.00 23.61 | L | C |
| | MOTA | 1358 | CZ | TYR L | | 19.179 | 19.382 | 23.884 | 1.00 31.64 | L | C |
| | MOTA | 1359 | OH | TYR L | 173 | 19.533 | 19.124 | 22.587 | 1.00 50.61 | L | 0 |
| | ATOM | 1360 | N | SER L | 174 | 16.172 | 20.261 | 30.396 | 1.00 32.25 | L | N |
| | MOTA | 1361 | CA | SER L | 174 | 15.932 | 20.103 | 31.810 | 1.00 33.25 | L | C |
| 55 | MOTA | 1362 | C | SER L | | 15.820 | 18.624 | 32.103 | 1.00 31.14 | L | C |
| | MOTA | 1363 | 0 | SER L | 174 | 15.363 | 17.840 | 31.270 | 1.00 35.74 | L | 0 |
| | ATOM | 1364 | CB | SER L | | 14.644 | 20.817 | 32.210 | 1.00 34.96 | L | С |
| | ATOM | 1365 | OG | SER L | | 14.723 | 22.191 | 31.872 | 1.00 44.21 | L | Ō |
| | ATOM | 1366 | N | MET L | | 16.264 | 18.235 | 33.283 | 1.00 32.45 | L | N |
| 60 | ATOM | 1367 | CA | MET L | | 16.185 | 16.848 | 33.665 | 1.00 33.65 | L | Ĉ |
| • | ATOM | 1368 | C | MET L | | 15.658 | 16.798 | 35.083 | 1.00 36.03 | L | Č |
| | ATOM | 1369 | ŏ | MET L | | 15.931 | 17.675 | 35.895 | 1.00 37.60 | L | ŏ |
| | ATOM | 1370 | CB | MET L | | 17.555 | 16.169 | 33.576 | 1.00 34.51 | r 1 | Č |
| | ATOM | 1371 | CG | MET L | | 18.065 | 15.622 | 34.890 | 1.00 34.31 | L | C |
| 65 | ATOM | 1372 | SD | MET L | | 18.885 | 14.022 | 34.685 | 1.00 50.79 | L | s |
| 00 | | 1372 | | MET L | | 17.718 | 12.956 | | 1.00 50.79 | r L | C |
| | ATOM | | CE | | | 14.872 | 15.769 | 35.395 | 1.00 31.77 | r r | |
| | ATOM | 1374 | N | SER L | | | | 35.352 | 1.00 38.28 | | N |
| | ATOM | 1375 | CA | SER L | | 14.285 | 15.553 | 36.650 | | L L | C |
| | ATOM | 1376 | С | SER L | T / O | 14.794 | 14.211 | 37.167 | 1.00 33.00 | Ţī | C |

| | ATOM ATOM ATOM | 1377 1378 1379 | O CB OG | SER L SER L SER L | 176 176 | 14.9 12.7 12.1 | 66 40 | 13.256 15.526 15.055 | 36.38 36.53 37.68 | 10 80 | 1.00 | 25.85 | L L | 0 C 0 |
|----|------------------------------|------------------------------|-----------------------|----------------------------------|--------------------------|------------------------------|-------------------|--------------------------------------|----------------------------------|----------------|----------------------|----------------------------------|------------------|-------------|
| 5 | ATOM ATOM ATOM ATOM | 1380 1381 1382 1383 | N CA C O | SER L | 177 177 177 177 | 15.0 15.5 14.7 14.5 | 09 87 | 14.137 12.887 12.492 13.325 | 38.4° 39.00 40.34 41.2° | 60 49 | 1.00 | 34.20 31.30 30.60 34.61 | L L L | 0 C N |
| 10 | ATOM ATOM ATOM | 1384 1385 1386 | CB OG N | SER L SER L THR L | 177 177 178 | 17.0 17.4 14.5 | 04 80 00 | 12.939 11.618 11.205 | 39.30 39.25 40.46 | 06 57 80 | 1.00 1.00 1.00 | 22.17 35.64 28.83 | L L L | С О И |
| | ATOM ATOM ATOM ATOM | 1387 1388 1389 1390 | CA C O CB | THR L THR L THR L | 178 178 | 13.7 14.3 14.5 12.3 | 78 27 | 10.744 9.497 8.460 10.452 | 41.6 42.2 41.6 41.2 | 87 44 | 1.00 1.00 | 28.12 33.56 34.19 29.07 | L L L L | 000 |
| 15 | ATOM ATOM ATOM | 1391 1392 1393 | | THR L | 178 178 | 11.7 11.5 14.7 | 00 26 17 | 11.620 10.050 9.609 | 40.73 42.53 43.5 | 26 20 65 | 1.00 1.00 1.00 | 34.69 38.66 37.13 | L L L | О С О |
| 20 | ATOM ATOM ATOM | 1394 1395 1396 1397 | CA C O CB | LEU L LEU L LEU L | 179 179 | 15.2 14.1 13.8 16.5 | .33 :03 | 8.478 8.072 8.813 8.852 | 44.3 45.2 46.2 45.0 | 94 19 | 1.00 | 37.36 38.67 46.22 38.33 | L L L L | 000 |
| | ATOM ATOM ATOM ATOM | 1398 1399 1400 | CG CD1 | LEU L | 179 179 | 16.9 16.8 18.3 | 37 37 | 7.711 6.398 7.964 | 46.0 45.2 46.5 | 13 65 | 1.00 1.00 | 39.81 36.12 42.75 | L L L | 2000 |
| 25 | MOTA MOTA MOTA | 1401 1402 1403 | N CA C | THR L THR L THR L | 180 180 | 13.5 12.4 13.0 | 78 17 | 6.905 6.453 5.573 | 45.0 45.9 47.0 | 47 59 | 1.00 | 40.70 46.91 | L L L | C C |
| 30 | ATOM ATOM ATOM ATOM | 1404 1405 1406 1407 | O CB OG1 CG2 | | 180 180 | 13.8 11.4 10.9 10.2 | 20 83 | 4.712 5.660 6.437 5.338 | 46.8 45.1 44.0 46.0 | 55 33 | 1.00 1.00 | 55.35 42.81 53.11 40.36 | L L L | 0000 |
| | ATOM ATOM ATOM | 1408 1409 1410 | N CA C | LEU L LEU L | 181 181 | 12.5 12.8 11.6 | 02 896 526 | 5.796 5.043 4.660 | 48.2 49.4 50.1 | 64 40 61 | 1.00 1.00 1.00 | 44.68 38.18 42.65 | L L L | C C M |
| 35 | ATOM ATOM ATOM ATOM | 1411 1412 1413 1414 | O CB CG | LEU L LEU L LEU L | 181 181 | 10.5 13.7 14.8 15.4 | 20 354 | 5.241 5.920 6.721 7.699 | 49.9 50.3 49.7 50.7 | 75 50 | 1.00 1.00 | 47.04 36.56 35.79 23.79 | L L L | 0000 |
| 40 | ATOM ATOM ATOM | 1415 1416 1417 | - | LEU L THR L THR L | 181 182 | 15.9 11.7 10.5 | 929 716 | 5.772 3.675 3.276 | 49.2 51.0 51.8 | 43 44 | 1.00 1.00 | 48.44 49.61 45.22 | L L L | C N C |
| 45 | ATOM ATOM ATOM | 1418 1419 1420 | C O CB | THR L THR L THR L | 182 182 | 10.6 11.7 10.7 | 717 733 | 4.266 4.776 1.838 | 53.0 53.3 52.4 | 36 23 | 1.00 1.00 | | L L L | 0 0 0 |
| 45 | MOTA MOTA MOTA MOTA | 1421 1422 1423 1424 | OG1 CG2 N CA | | 182 183 | 11.8 10.9 9.5 9.4 | 914 507 | 1.786 0.832 4.540 5.472 | 53.2 51.3 53.6 54.7 | 08 62 | 1.00 | 53.75 50.23 45.54 48.11 | L L L | N C |
| 50 | ATOM ATOM ATOM | 1425 1426 1427 | C O CB | LYS L LYS L | 183 183 183 | 10.4 10.8 8.0 | 181 369 049 | 5.104 5.951 5.521 | 55.8 56.7 55.3 | 98 11 87 | 1.00 1.00 1.00 | 51.20 49.30 43.28 | L L L | 0 0 |
| 55 | MOTA MOTA MOTA MOTA | 1428 1429 1430 1431 | CG CD CE NZ | LYS L LYS L LYS L LYS L | 183 183 | 7.8 6.6 6.7 5.6 | 517 771 | 6.643 6.417 5.152 4.941 | 56.3 57.2 58.0 59.0 | 55 89 | 1.00 1.00 | 40.50 66.92 77.94 73.24 | L L L L | И С С |
| 33 | ATOM ATOM ATOM | 1432 1433 1434 | N CA C | ASP L ASP L ASP L | 184 184 | 10.9 11.8 13.2 | 913 311 | 3.843 3.416 3.930 | 55.9 56.9 56.7 | 17 84 63 | 1.00 1.00 1.00 | 52.45 53.02 48.73 | L L L | С С И |
| 60 | MOTA MOTA MOTA | 1435 1436 1437 | O CB CG | ASP L ASP L | 184 184 | 13.8 11.8 10.7 | 309 705 | 4.649 1.885 1.407 | 57.5 57.0 57.9 | 27 60 | 1.00 | 51.85 57.50 71.44 | L L L | 0000 |
| 65 | MOTA MOTA MOTA MOTA | 1438 1439 1440 1441 | | ASP L ASP L GLU L GLU L | 184 185 | 10.0 10.4 13.8 15.1 | 160 332 | 2.257 0.205 3.497 3.944 | 58.6 58.0 55.6 55.3 | 21 35 | 1.00 | 66.16 81.91 43.10 42.13 | L L L | С 0 0 |
| | MOTA MOTA MOTA | 1442 1443 1444 | C O CB | GLU L GLU L | 185 185 185 | 15.2 16.2 15.5 | 286 246 566 | 5.470 6.060 3.406 | 55.3 55.8 53.9 | 34 13 43 | 1.00 1.00 1.00 | 45.22 50.22 43.08 | L L L | С С |
| | MOTA | 1445 | CG | GLU L | 185 | 16.9 | 145 | 3.889 | 53.4 | 92 | T.00 | 22.88 | L | С |

| | ATOM | 1446 | CD GLU L | 185 | 18.015 | 3.077 | 54.186 | 1.00 39.62 | L | С |
|-----|---------|--------------|-----------|-----|--------|--------|--------|-------------------|--------------|----------|
| | - | | | | | | | | | |
| | ATOM | 1447 | | 185 | 17.699 | 2.384 | 55.144 | 1.00 47.97 | L | 0 |
| | ATOM | 1448 | OE2 GLU L | 185 | 19.166 | 3.140 | 53.756 | 1.00 53.07 | L | 0 |
| | ATOM | 1449 | N TYR L | 186 | 14.262 | 6.113 | 54.741 | 1.00 42.12 | L | N |
| - | | | | | | | | | | |
| 5 | MOTA | 1450 | CA TYR L | | 14.233 | 7.570 | 54.754 | 1.00 40.44 | L | C |
| | MOTA | 1451 | C TYR L | 186 | 14.366 | 8.112 | 56.179 | 1.00 40.33 | L | C |
| | ATOM | 1452 | O TYR L | | 15.068 | 9.081 | 56.442 | 1.00 46.64 | | |
| | | | | | | | | | L | 0 |
| | MOTA | 1453 | CB TYR L | 186 | 12.909 | 8.028 | 54.140 | 1.00 41.32 | L | С |
| | ATOM | 1454 | CG TYR L | 186 | 12.823 | 9.514 | 54.177 | 1.00 38.85 | L | C |
| 40 | | | | | | | | | | č |
| 10 | MOTA | 1455 | CD1 TYR L | | 13.822 | 10.281 | 53.582 | 1.00 29.72 | L | C |
| | MOTA | 1456 | CD2 TYR L | 186 | 11.778 | 10.146 | 54.851 | 1.00 37.41 | L | С |
| | ATOM | 1457 | CE1 TYR L | | 13.779 | 11.665 | 53.663 | 1.00 28.90 | L | Ċ |
| | | | | | | | | | | _ |
| | MOTA | 1458 | CE2 TYR L | 186 | 11.740 | 11.529 | 54.940 | 1.00 32.41 | L | C |
| | MOTA | 1459 | CZ TYR L | 186 | 12.739 | 12.287 | 54.358 | 1.00 30.10 | L | C |
| 45 | | 1460 | OH TYR L | | 12.710 | 13.665 | 54.446 | | | |
| 15 | MOTA | | | | | | | | L | 0 |
| | MOTA | 1461 | N GLU L | 187 | 13.695 | 7.510 | 57.147 | 1.00 44.49 | L | N |
| | MOTA | 1462 | CA GLU L | 187 | 13.790 | 7.981 | 58.520 | 1.00 46.87 | L | C |
| | | | | | | | | | | |
| | ATOM | 1463 | C GLU L | | 15.085 | 7.549 | 59.202 | 1.00 48.70 | L | C |
| | ATOM | 1464 | O GLU L | 187 | 15.510 | 8.156 | 60.176 | 1.00 50.91 | L | 0 |
| 20 | ATOM | 1465 | CB GLU L | 187 | 12.573 | 7.503 | 59.306 | 1.00 42.22 | L | C |
| 20 | | | | | | | | | | ~ |
| | ATOM | 1466 | CG GLU L | | 11.368 | 8.395 | 59.085 | 1.00 62.96 | L | C |
| | ATOM | 1467 | CD GLU L | 187 | 10.044 | 7.666 | 59.223 | 1.00 86.23 | L | C |
| | ATOM | 1468 | OE1 GLU L | 187 | 9.906 | 6.832 | 60.150 | 1.00 80.19 | L | 0 |
| | | | | | | | | | | |
| | MOTA | 1469 | | 187 | 9.135 | 7.943 | 58.405 | 1.00 94.40 | L | 0 |
| 25 | ATOM | 1470 | N ARG L | 188 | 15.725 | 6.512 | 58.675 | 1.00 46.28 | L | N |
| | ATOM | 1471 | CA ARG L | | 16.965 | 6.029 | 59.252 | 1.00 44.52 | L | C |
| | | | | | | | | | | _ |
| | MOTA | 1472 | C ARG L | 188 | 18.131 | 6.934 | 58.890 | 1.00 46.66 | L | C |
| | MOTA | 1473 | O ARG L | 188 | 19.235 | 6.767 | 59.406 | 1.00 52.73 | L | 0 |
| | | 1474 | | | 17.269 | 4.623 | 58.754 | | | |
| | ATOM | | | | | | | 1.00 48.29 | L | C |
| 30 | MOTA | 1475 | CG ARG L | 188 | 16.216 | 3.585 | 59.050 | 1.00 58.26 | L | С |
| | MOTA | 1476 | CD ARG L | 188 | 16.723 | 2.255 | 58.545 | 1.00 65.07 | L | С |
| | | | | | | | | | | |
| | ATOM | 1477 | NE ARG L | | 18.049 | 2.009 | 59.098 | 1.00 63.58 | L | N |
| | ATOM | 1478 | CZ ARG L | 188 | 18.257 | 1.507 | 60.307 | 1.00 66.13 | L | C |
| | ATOM | 1479 | NH1 ARG L | 188 | 17.220 | 1.187 | 61.069 | 1.00 54.33 | L | N |
| 0.5 | | | | | | | | | | |
| 35 | ATOM | 1480 | NH2 ARG L | | 19.496 | 1.357 | 60.761 | 1.00 56.10 | L | N |
| | ATOM | 1481 | N HIS L | 189 | 17.890 | 7.882 | 57.993 | 1.00 44.20 | L | N |
| | ATOM | 1482 | CA HIS L | | 18.897 | 8.764 | 57.427 | 1.00 42.62 | L | С |
| | | | | | | | | | | |
| | ATOM | 1483 | C HIS L | 189 | 18.505 | 10.231 | 57.645 | 1.00 45.89 | L | C |
| | ATOM | 1484 | O HIS L | 189 | 17.414 | 10.556 | 58.093 | 1.00 46.26 | L | 0 |
| 40 | ATOM | 1485 | | 189 | 19.037 | 8.429 | 55.935 | 1.00 45.73 | L | Č |
| 40 | | | | | | | | | | Č |
| | MOTA | 1486 | CG HIS L | 189 | 19.693 | 7.071 | 55.785 | 1.00 40.19 | L | С |
| | ATOM | 1487 | ND1 HIS L | 189 | 20.953 | 6.813 | 56.208 | 1.00 51.00 | L | N |
| | ATOM | 1488 | | 189 | 19.093 | 5.857 | 55.443 | 1.00 59.83 | L | Ĉ |
| | | | | | | | | | | |
| | MOTA | 1489 | | 189 | 21.100 | 5.477 | 56.140 | 1.00 47.50 | L | С |
| 45 | ATOM | 1490 | NE2 HIS L | 189 | 20.000 | 4.877 | 55.685 | 1.00 61.66 | L | N |
| | ATOM | 1491 | | 190 | 19.455 | 11.138 | 57.354 | 1.00 50.73 | L | N |
| | | | | | | | | | | |
| | ATOM | 1492 | | 190 | 19.221 | 12.519 | 57.748 | 1.00 55.47 | L | C |
| | ATOM | 1493 | C ASN L | 190 | 19.747 | 13.531 | 56.728 | 1.00 53.43 | L | С |
| | MOTA | 1494 | O ASN L | | 19.229 | 14.627 | 56.573 | 1.00 62.98 | L | 0 |
| 50 | | | | | | | | | | |
| 50 | ATOM | 1495 | CB ASN L | | 19.865 | 12.710 | 59.122 | 1.00 57.60 | L | C |
| | ATOM | 1496 | CG ASN L | 190 | 20.194 | 14.160 | 59.395 | 1.00 71.59 | \mathbf{L} | C |
| | ATOM | 1497 | OD1 ASN L | 190 | 19.343 | 14.991 | 59.710 | 1.00 84.26 | L | 0 |
| | | | | | | | | | | |
| | ATOM | 1498 | ND2 ASN L | | 21.512 | 14.435 | 59.365 | 1.00 74.56 | L | N |
| | ATOM | 1499 | N SER L | 191 | 20.835 | 13.144 | 56.039 | 1.00 48.57 | L | N |
| 55 | ATOM | 1500 | CA SER L | | 21.348 | 13.985 | 54.965 | 1.00 48.43 | L | Ĉ |
| 55 | | | | | | | | | | |
| | ATOM | 1501 | C SER L | | 21.082 | 13.358 | 53.597 | 1.00 48.76 | L | C |
| | MOTA | 1502 | O SER L | 191 | 21.648 | 12.330 | 53.245 | 1.00 49.95 | L | 0 |
| | | 1503 | | | 22.855 | 14.138 | 55.160 | | | |
| | MOTA | | CB SER L | | | | | 1.00 48.79 | Ē | C |
| | ATOM | 1504 | OG SER L | | 23.356 | 15.077 | 54.204 | 1.00 58.59 | L | 0 |
| 60 | ATOM | 1505 | N TYR L | 192 | 20.292 | 14.056 | 52.790 | 1.00 48.13 | L | N |
| | ATOM | 1506 | | | 20.040 | 13.643 | 51.414 | 1.00 45.11 | | Ĉ |
| | | | CA TYR L | | | | | | L | ٢ |
| | MOTA | 1507 | C TYR L | 192 | 20.650 | 14.655 | 50.465 | 1.00 42.96 | L | C |
| | ATOM | 1508 | O TYR L | | 20.321 | 15.835 | 50.508 | 1.00 38.34 | L | 0 |
| | | | | | | | | | | \simeq |
| | ATOM | 1509 | CB TYR L | | 18.537 | 13.507 | 51.187 | 1.00 45.18 | L | C |
| 65 | ATOM | 1510 | CG TYR L | 192 | 17.948 | 12.438 | 52.077 | 1.00 42.77 | L | C |
| | ATOM | 1511 | CD1 TYR L | | 17.896 | 12.600 | 53.459 | 1.00 22.56 | L | C |
| | | | | | | | | | | ~ |
| | ATOM | 1512 | CD2 TYR L | | 17.518 | 11.239 | 51.546 | 1.00 38.31 | L | C |
| | ATOM | 1513 | CE1 TYR L | 192 | 17.442 | 11.597 | 54.275 | 1.00 25.40 | L | C |
| | ATOM | 1514 | CE2 TYR L | | 17.061 | 10.231 | 52.357 | 1.00 44.54 | L | Č |
| | 111 011 | - | J. 111 L | | 11.001 | _U.2JI | 22.337 | 1 1.04 | ш | • |
| | | | | | | | | | | |

| | MOTA | 1515 | CIT | TYR L | 100 | 17 000 | 10 410 | E2 710 | 1 00 27 00 | ~ | ~ |
|------------|--------------|--------------|-------------|----------------|-----|------------------|------------------|------------------|--------------------------|--------|-----|
| | ATOM | 1516 | CZ OH | TYR L | | 17.026 16.567 | 10.412 | 53.718 | 1.00 37.89 | I | - |
| | MOTA | 1517 | N | THR L | | 21.551 | 9.387 14.175 | 54.500 49.614 | 1.00 32.01 1.00 45.21 | Ţ | |
| | ATOM | 1518 | CA | THR L | | 22.250 | 15.023 | 48.673 | 1.00 45.21 | I | |
| 5 | MOTA | 1519 | C | THR L | | 22.230 | 14.665 | 47.212 | 1.00 44.18 | I I | |
| • | ATOM | 1520 | õ | THR L | | 22.003 | 13.501 | 46.824 | 1.00 45.22 | L | |
| | MOTA | 1521 | СВ | THR L | | 23.756 | 15.056 | 48.993 | 1.00 47.97 | I | |
| | ATOM | 1522 | OG1 | | | 24.036 | 16.172 | 49.837 | 1.00 49.86 | I | |
| | MOTA | 1523 | CG2 | | | 24.587 | 15.168 | 47.717 | 1.00 56.55 | Ī | |
| 10 | ATOM | 1524 | N | CYS L | | 21.958 | 15.708 | 46.407 | 1.00 45.78 | Ī | |
| . • | ATOM | 1525 | CA | CYS L | | 21.804 | 15.595 | 44.971 | 1.00 45.45 | I. | |
| | ATOM | 1526 | C | CYS L | | 22.924 | 16.422 | 44.319 | 1.00 41.02 | ī | |
| | ATOM | 1527 | O | CYS L | | 23.002 | 17.627 | 44.525 | 1.00 44.64 | Ĩ | |
| | ATOM | 1528 | CB | CYS L | | 20.411 | 16.118 | 44.584 | 1.00 45.40 | Ī | |
| 15 | ATOM | 1529 | SG | CYS L | | 20.133 | 16.300 | 42.804 | 1.00 69.21 | Ī | |
| | MOTA | 1530 | N | GLU L | 195 | 23.798 | 15.772 | 43.551 | 1.00 39.80 | ī | |
| | ATOM | 1531 | CA | GLU L | 195 | 24.909 | 16.467 | 42.893 | 1.00 42.67 | I | |
| | MOTA | 1532 | С | GLU L | 195 | 24.837 | 16.414 | 41.366 | 1.00 41.70 | I | |
| | ATOM | 1533 | 0 | GLU L | 195 | 24.670 | 15.347 | 40.782 | 1.00 36.42 | I | |
| 20 | MOTA | 1534 | CB | GLU L | 195 | 26.246 | 15,869 | 43.326 | 1.00 46.01 | I | |
| | MOTA | 1535 | CG | GLU L | | 26.367 | 15.583 | 44.810 | 1.00 64.77 | I | |
| | ATOM | 1536 | CD | GLU L | | 27.797 | 15.282 | 45.221 | 1.00 73.00 | L | |
| | ATOM | 1537 | OE1 | | | 28.569 | 14.796 | 44.364 | 1.00 56.32 | I | 0 |
| | ATOM | 1538 | | GLU L | | 28.145 | 15.522 | 46.401 | 1.00 72.72 | L | . 0 |
| 25 | MOTA | 1539 | N | ALA L | | 24.990 | 17.568 | 40.723 | 1.00 40.13 | I | |
| | ATOM | 1540 | CA | ALA L | | 24.938 | 17.639 | 39.267 | 1.00 42.38 | L | |
| | MOTA | 1541 | C | ALA L | | 26.315 | 17.873 | 38.670 | 1.00 47.42 | L | |
| | ATOM | 1542 | 0 | ALA L | | 27.060 | 18.740 | 39.123 | 1.00 45.43 | L | |
| 00 | ATOM | 1543 | CB | ALA L | | 23.990 | 18.747 | 38.827 | 1.00 40.85 | L | |
| 30 | ATOM | 1544 | N | THR L | | 26.644 | 17.096 | 37.642 | 1.00 54.27 | L | |
| | ATOM | 1545 | CA | THR L | | 27.938 | 17.210 | 36.976 | 1.00 56.97 | L | |
| | ATOM | 1546 | C | THR L | | 27.707 | 17.576 | 35.519 | 1.00 52.12 | L | |
| | ATOM | 1547 | 0 | THR L | | 27.154 | 16.795 | 34.756 | 1.00 54.86 | L | _ |
| 35 | MOTA MOTA | 1548 1549 | | THR L | | 28.723 | 15.879 | 37.032 | 1.00 60.44 | L | |
| 33 | | | OG1 | | | 28.656 | 15.329 | 38.357 | 1.00 55.79 | L | |
| | ATOM ATOM | 1550 1551 | | THR L | | 30.177 | 16.113 | 36.668 | 1.00 66.98 | L | - |
| | ATOM | 1552 | N CA | HIS L | | 28.135 27.958 | 18.770 19.255 | 35.141 33.783 | 1.00 52.54 | L | |
| | ATOM | 1553 | C | HIS L | | 29.244 | 19.233 | 33.703 | 1.00 49.05 | L | - |
| 40 | ATOM | 1554 | Ö | HIS L | | 29.244 | 20.490 | 34.143 | 1.00 50.31 1.00 51.38 | L | |
| -10 | ATOM | 1555 | СВ | HIS L | | 26.769 | 20.226 | 33.750 | 1.00 31.38 | L | |
| | ATOM | 1556 | CG | | 198 | 26.396 | 20.692 | 32.376 | 1.00 48.32 | I. | |
| | MOTA | 1557 | | HIS L | | 26.284 | 19.834 | 31.302 | 1.00 55.30 | L | |
| | ATOM | 1558 | | HIS L | | 26.068 | 21.921 | 31.912 | 1.00 45.28 | L | |
| 45 | MOTA | 1559 | | HIS L | | 25.904 | 20.515 | 30.236 | 1.00 64.72 | L | |
| | ATOM | 1560 | | HIS L | | 25.764 | 21.783 | 30.579 | 1.00 54.41 | L | |
| | ATOM | 1561 | N | LYS L | | 29.501 | 19.917 | 32.025 | 1.00 54.03 | L | |
| | MOTA | 1562 | CA | LYS L | | 30.708 | 20.526 | 31.484 | 1.00 53.00 | L | |
| | ATOM | 1563 | С | LYS L | | 30.883 | 21.998 | 31.851 | 1.00 55.09 | Ŀ | |
| 50 | ATOM | 1564 | 0 | LYS L | 199 | 31.990 | 22.529 | 31.768 | 1.00 59.80 | L | |
| | ATOM | 1565 | CB | LYS L | | 30.735 | 20.383 | 29.965 | 1.00 51.53 | L | |
| | MOTA | 1566 | CG | LYS L | | 29.631 | 21.136 | 29.262 | 1.00 54.50 | L | |
| | ATOM | 1567 | $^{\rm CD}$ | LYS L | | 29.886 | 21.211 | 27.768 | 1.00 69.27 | L | |
| | MOTA | 1568 | CE | LYS L | | 31.152 | 21.991 | 27.463 | 1.00 89.21 | L | |
| 5 5 | ATOM | 1569 | NZ | LYS L | | 31.310 | 22.208 | 25.993 | 1.00 98.42 | L | N |
| | MOTA | 1570 | N | THR L | | 29.807 | 22.662 | 32.256 | 1.00 52.50 | L | N |
| | MOTA | 1571 | CA | THR L | | 29.900 | 24.074 | 32.613 | 1.00 55.94 | L | С |
| | ATOM | 1572 | C | THR L | | 30.727 | 24.351 | 33.871 | 1.00 59.72 | L | |
| 66 | ATOM | 1573 | 0 | THR L | | 30.788 | 25.486 | 34.347 | 1.00 66.15 | L | |
| 60 | ATOM | 1574 | CB | THR L | | 28.513 | 24.686 | 32.803 | 1.00 48.37 | L | |
| | MOTA | 1575 | OG1 | | | 27.731 | 23.834 | 33.643 | 1.00 59.04 | L | |
| | ATOM | 1576 | | THR L | | 27.830 | 24.864 | 31.473 | 1.00 53.65 | L | |
| | ATOM | 1577 | N | SER L | | 31.359 | 23.313 | 34.407 | 1.00 62.13 | L | |
| GE. | ATOM | 1578 | CA | SER L | | 32.188 | 23.453 | 35.599 | 1.00 63.39 | L | |
| 65 | MOTA | 1579 | C | SER L | | 32.916 | 22.159 | 35.938 | 1.00 61.33 | Ŀ | |
| | ATOM | 1580 | O CB | SER L | | 32.604 | 21.089 | 35.409 | 1.00 60.64 | L | |
| | MOTA MOTA | 1581 1582 | CB | SER L | | 31.341 | 23.885 | 36.792 | 1.00 61.74 | L | |
| | ATOM | 1582 | OG N | SER L THR L | | 30.356 33.892 | 22.917 22.273 | 37.086 | 1.00 76.78 | L | _ |
| | TT OIL | 100 | τA | 7 111/ TJ | 404 | 55.054 | 44.413 | 36.828 | 1.00 63.77 | L | N |

| | MOTA | 1584 | CA THR L 2 | | 21.131 | 37.267 | 1.00 68.80 | Ŀ | C |
|----|--------------|--------------|-------------------------|---------------------|------------------|------------------|--------------------------|-----------------------|--------|
| | ATOM | 1585 1586 | C THR L 2 O THR L 2 | 34.141 32 34.216 | 20.557 19.353 | 38.568 38.808 | 1.00 69.42 1.00 69.26 | L L | C O |
| | ATOM ATOM | 1585 | | 34.216 36.158 | 21.536 | 37.473 | 1.00 72.06 | L | C |
| 5 | ATOM | 1588 | OG1 THR L 2 | | 22.783 | 38.188 | 1.00 66.18 | L | ō |
| J | ATOM | 1589 | CG2 THR L 2 | | 21.665 | 36.123 | 1.00 68.77 | L | C |
| | ATOM | 1590 | N SER L 2 | | 21.427 | 39.409 | 1.00 71.13 | L | N |
| | MOTA | 1591 | CA SER L 2 | | 20.997 | 40.673 | 1.00 74.47 | L | C |
| | MOTA | 1592 | C SER L 2 | | 20.732 | 40.462 | 1.00 71.15 | L | C |
| 10 | MOTA | 1593 | O SER L 2 | | 21.524 | 39.832 | 1.00 69.36 | L | 0 |
| | ATOM | 1594 | CB SER L 2 | | 22.078 23.358 | 41.743 41.274 | 1.00 76.75 1.00 81.99 | L L | C O |
| | ATOM ATOM | 1595 1596 | OG SER L 2 N PRO L 2 | | 19.605 | 40.979 | 1.00 67.69 | P T | И |
| | ATOM | 1597 | CA PRO L 2 | | 19.297 | 40.808 | 1.00 62.61 | Ľ | Ĉ |
| 15 | ATOM | 1598 | | 204 28.712 | 20.237 | 41.606 | 1.00 56.97 | L | Ċ |
| | ATOM | 1599 | O PRO L 2 | | 20.610 | 42.722 | 1.00 62.74 | L | 0 |
| | MOTA | 1600 | CB PRO L 2 | | 17.853 | 41.296 | 1.00 56.97 | L | С |
| | MOTA | 1601 | CG PRO L 2 | | 17.821 | 42.393 | 1.00 66.29 | T | C |
| | ATOM | 1602 | | 204 31.687 | 18.554 | 41.765 | 1.00 70.41 | Ŀ | C |
| 20 | MOTA | 1603 | _ | 205 27.588 | 20.627 21.509 | 41.016 41.678 | 1.00 51.68 1.00 46.32 | L L | C N |
| | ATOM ATOM | 1604 1605 | CA ILE L 2 C ILE L 2 | | 20.662 | 42.696 | 1.00 45.80 | r r | č |
| | ATOM | 1606 | O ILE L 2 | | 19.801 | 42.333 | 1.00 40.05 | L | ŏ |
| | ATOM | 1607 | CB ILE L 2 | | 22.094 | 40.672 | 1.00 45.71 | L | C |
| 25 | MOTA | 1608 | CG1 ILE L 2 | 205 26.431 | 22.817 | 39.578 | 1.00 42.60 | . L | С |
| | ATOM | 1609 | CG2 ILE L 2 | | 23.039 | 41.371 | 1.00 48.15 | Ŀ | C |
| | MOTA | 1610 | CD1 ILE L 2 | | 23.579 | 38.620 | 1.00 57.30 | L | C |
| | MOTA | 1611 | N VAL L 2 CA VAL L 2 | | 20.909 20.118 | 43.972 45.017 | 1.00 42.27 1.00 45.01 | L L | C N |
| 30 | ATOM ATOM | 1612 1613 | CA VAL L 2 C VAL L 2 | | 20.803 | 45.743 | 1.00 43.48 | L | C |
| 30 | ATOM | 1614 | O VAL L 2 | | 21.965 | 46.114 | 1.00 54.37 | L | ō |
| | MOTA | 1615 | CB VAL L 2 | | 19.666 | 46.058 | 1.00 42.29 | L | С |
| | ATOM | 1616 | CG1 VAL L 2 | | 18.715 | 47.046 | 1.00 48.63 | L | С |
| | MOTA | 1617 | CG2 VAL L 2 | | 18.992 | 45.358 | 1.00 38.47 | Ŀ | C |
| 35 | MOTA | 1618 | N LYS L 2 | | 20.064 | 45.931 | 1.00 41.43 | L | Ŋ |
| | ATOM | 1619 | CA LYS L 2 | | 20.569 | 46.631 | 1.00 45.71 1.00 45.03 | L L | C C |
| | MOTA | 1620 1621 | C LYS L 2 O LYS L 2 | | 19.478 18.302 | 47.584 47.238 | 1.00 45.03 | L | Ö |
| | MOTA MOTA | 1622 | CB LYS L 2 | | 20.886 | 45.654 | 1.00 49.37 | L | č |
| 40 | ATOM | 1623 | CG LYS L 2 | | 22.063 | 44.750 | 1.00 55.07 | L | Ċ |
| | MOTA | 1624 | CD LYS L 2 | | 23.357 | 45.532 | 1.00 64.96 | L | C |
| | MOTA | 1625 | CE LYS L 2 | | 24.505 | 44.598 | 1.00 71.81 | L | C |
| | MOTA | 1626 | NZ LYS L 2 | | 25.798 | 45.310 | 1.00 78.53 | Ţ | N |
| 4= | ATOM | 1627 | N SER L 2 | | 19.859 | 48.787 49.747 | 1.00 44.02 1.00 49.80 | L L | N C |
| 45 | MOTA MOTA | 1628 1629 | CA SER L 2 C SER L 2 | | 18.856 19.432 | 50.931 | 1.00 49.80 | L L | Č |
| | ATOM | 1630 | O SER L 2 | | 20.627 | 51.198 | 1.00 53.70 | Ľ | õ |
| | MOTA | 1631 | CB SER L 2 | | 18.103 | 50.243 | 1.00 53.51 | L | C |
| | MOTA | 1632 | OG SER L 2 | 208 23.078 | 19.005 | 50.763 | 1.00 59.07 | Ŀ | 0 |
| 50 | MOTA | 1633 | N PHE L 2 | | 18.550 | 51.646 | 1.00 51.91 | Ŀ | N |
| | ATOM | 1634 | CA PHE L 2 | | 18.933 | 52.822 | 1.00 51.34 | L | C |
| | MOTA | 1635 | C PHE L 2 | | 17.894 | 53.923 53.688 | 1.00 49.64 1.00 54.59 | L L | C O |
| | ATOM ATOM | 1636 1637 | O PHE L 2 CB PHE L 2 | | 16.815 19.038 | 52.464 | 1.00 34.39 | L | č |
| 55 | ATOM | 1638 | CG PHE L 2 | | 17.728 | 52.091 | 1.00 46.90 | $ar{	ilde{	ilde{L}}}$ | č |
| 00 | ATOM | 1639 | CD1 PHE L 2 | | 16.836 | 53.064 | 1.00 37.57 | L | C |
| | ATOM | 1640 | CD2 PHE L 2 | | 17.380 | 50.761 | 1.00 53.34 | L | C |
| | ATOM | 1641 | CE1 PHE L 2 | | 15.625 | 52.714 | 1.00 47.31 | Ē | C |
| | MOTA | 1642 | CE2 PHE L 2 | | 16.172 | 50.411 | 1.00 36.37 | L | C |
| 60 | ATOM | 1643 | CZ PHE L 2 | 209 15.469 | 15.296 | 51.386 | 1.00 34.65 | ь Г | C |
| | MOTA | 1644 | N ASN L 2 | | 18.228 17.302 | 55.131 56.242 | 1.00 49.60 1.00 46.61 | L | C N |
| | MOTA MOTA | 1645 1646 | CA ASN L 2 C ASN L 2 | | 17.008 | 56.761 | 1.00 48.63 | L | Ċ |
| | MOTA | 1647 | O ASN L 2 | | 17.912 | 57.130 | 1.00 43.72 | L | õ |
| 65 | MOTA | 1648 | CB ASN L | | 17.888 | 57.343 | 1.00 42.76 | L | С |
| - | MOTA | 1649 | CG ASN L 2 | 210 20.935 | 17.681 | 57.073 | 1.00 60.02 | L | С |
| | MOTA | 1650 | OD1 ASN L | | 17.059 | 57.864 | 1.00 69.23 | L | O |
| | MOTA | 1651 | ND2 ASN L | | 18.185 | 55.935 | 1.00 75.72 | L L | N |
| | ATOM | 1652 | N ARG L | 211 16.835 | 15.732 | 56.762 | 1.00 50.53 | n | 7/4 |

| | ATOM | 1653 | CA | ARG L | 211 | 15.531 | 15.302 | 57.231 | 1.00 54.11 | | т | α |
|-------------|------|------|------------------|-------|--------|---------|--------|---------|------------|---|--------|----------|
| | | | | | | | | | | | L | C |
| | MOTA | 1654 | С | ARG L | | 15.280 | 15.835 | 58.631 | 1.00 62.11 | | L | C |
| | MOTA | 1655 | 0 | ARG L | 211 | 14.147 | 16.169 | 58.983 | 1.00 63.88 | | L | 0 |
| | MOTA | 1656 | CB | ARG L | 211 | 15.468 | 13.781 | 57.247 | 1.00 53.56 | | L | C |
| 5 | ATOM | 1657 | ĊĠ | ARG L | | 14.114 | 13.211 | 57.586 | 1.00 44.47 | | | |
| 5 | | | | | | | | | | | L | C |
| | ATOM | 1658 | $^{\mathrm{CD}}$ | ARG L | | 14.210 | 11.713 | 57.614 | 1.00 54.91 | | L | C |
| | ATOM | 1659 | NE | ARG L | 211 | 15.231 | 11.291 | 58.565 | 1.00 58.23 | | L | N |
| | MOTA | 1660 | CZ | ARG L | | 15.003 | 11.066 | 59.855 | 1.00 72.82 | | _ L | C |
| | | | | | | | | | | | | |
| | ATOM | 1661 | | ARG L | | 13.779 | 11.217 | 60.349 | 1.00 73.06 | | L | N |
| 10 | ATOM | 1662 | NH2 | ARG L | 211 | 16.001 | 10.703 | 60.653 | 1.00 62.59 | | L | N |
| | MOTA | 1663 | | ARG L | | 16.349 | 15.915 | 59.421 | 1.00 69.05 | | _ L | Ö |
| | | | 0211 | | | 10.545 | 10.010 | JJ. 421 | 1.00 05.05 | | | U |
| | TER | 1664 | | ARG L | | | | | | | | |
| | ATOM | 1665 | N | GLU H | 1 | -11.229 | 28.751 | 10.621 | 1.00 71.36 | | H | Ν |
| | ATOM | 1666 | ÇA | GLU H | 1 | -10.037 | 28.156 | 11.214 | 1.00 65.32 | | H | C |
| 15 | | 1667 | | GLU H | | -10.186 | 26.642 | 11.378 | | | | |
| 15 | MOTA | | C | | | | | | 1.00 58.26 | | H | C |
| | ATOM | 1668 | 0 | GLU H | 1 | -10.717 | 26.147 | 12.364 | 1.00 57.65 | | H | 0 |
| | ATOM | 1669 | CB | GLU H | 1 | -9.807 | 28.808 | 12.578 | 1.00 63.19 | | H | C |
| | ATOM | 1670 | CG | GLU H | | -9.166 | 27.849 | 13.582 | 1.00 71.03 | | H | Č |
| | | | | | | | | | | | | |
| | ATOM | 1671 | $^{\rm CD}$ | GLU H | 1 | -9.800 | 28.047 | 14.940 | 1.00 87.73 | | H | С |
| 20 | MOTA | 1672 | OE1 | GLU H | 1 | -9.507 | 29.044 | 15.584 | 1.00 95.88 | | H | 0 |
| | MOTA | 1673 | OE2 | GLU H | 1 | -10.586 | 27.192 | 15.346 | 1.00 96.84 | | H | 0 |
| | | 1674 | - | | | | | | | | | |
| | MOTA | | N | VAL H | | -9.728 | 25.874 | 10.404 | 1.00 56.34 | | | N |
| | MOTA | 1675 | ca | VAL H | 2 | -9.825 | 24.427 | 10.381 | 1.00 45.11 | | H | С |
| | ATOM | 1676 | С | VAL H | 2 | -9.533 | 23.838 | 11.759 | 1.00 40.35 | | H | C |
| 25 | ATOM | 1677 | ŏ | VAL H | | -8.616 | 24.234 | 12.465 | 1.00 44.32 | | | |
| 25 | | | | | | | | | | | H | 0 |
| | ATOM | 1678 | CB | VAL H | | -8.839 | 23.903 | 9.338 | 1.00 46.79 | | H | С |
| | MOTA | 1679 | CG1 | VAL H | 2 | -8.720 | 22.384 | 9.446 | 1.00 37.72 | | H | C |
| | ATOM | 1680 | CG2 | VAL H | | -9.339 | 24.265 | 7.948 | 1.00 32.94 | | H | Č |
| | | | | | | | | | | | | |
| | MOTA | 1681 | N | LYS H | | -10.391 | 22.889 | 12.155 | 1.00 39.63 | | H | N |
| 30 | MOTA | 1682 | $^{\rm CA}$ | LYS H | 3 | -10.299 | 22.350 | 13.496 | 1.00 40.75 | | H | C |
| | MOTA | 1683 | С | LYS H | 3 | -10.578 | 20.850 | 13.492 | 1.00 38.29 | | H | C |
| | MOTA | 1684 | ŏ | LYS H | | -11.632 | 20.381 | 13.091 | 1.00 46.18 | | | |
| | | | | | | | | | | | H | 0 |
| | ATOM | 1685 | $^{\mathrm{CB}}$ | LYS H | | -11.363 | 23.068 | 14.323 | 1.00 42.35 | | H | C |
| | MOTA | 1686 | CG | LYS H | 3 | -11.099 | 23.026 | 15.829 | 1.00 53.48 | | H | C |
| 35 | ATOM | 1687 | CD | LYS H | | -12.072 | 23.935 | 16.584 | 1.00 97.53 | | H | C |
| 00 | | | | | | | | | | | | |
| | ATOM | 1688 | CE | LYS H | | -12.025 | 23.731 | 18.102 | 1.00126.21 | | H | C |
| | MOTA | 1689 | NZ | LYS H | 3 | -12.982 | 24.629 | 18.743 | 1.00139.14 | | H | N |
| | ATOM | 1690 | N | LEU H | | -9.564 | 20.084 | 13.906 | 1.00 36.69 | | H | N |
| | | | | | | | | | | | | |
| | MOTA | 1691 | $^{\rm CA}$ | LEU H | | -9.766 | 18.650 | 13.973 | 1.00 31.82 | | H | С |
| 40 | ATOM | 1692 | С | LEU H | 4 | -9.672 | 18.147 | 15.411 | 1.00 36.95 | | H | C |
| | MOTA | 1693 | 0 | LEU H | 4 | -8.625 | 18.185 | 16.044 | 1.00 35.06 | • | H | 0 |
| | ATOM | 1694 | ČВ | LEU H | | -8.723 | 17.970 | 13.083 | 1.00 27.41 | | | |
| | | | | | | | | | | | H | C |
| | ATOM | 1695 | CG | LEU H | | -8.916 | 18.323 | 11.603 | 1.00 23.69 | | H | C |
| | MOTA | 1696 | CD1 | LEU H | 4 | -7.819 | 17.725 | 10.718 | 1.00 29.88 | | H | C |
| 45 | MOTA | 1697 | | LEU H | | -10.246 | 17.817 | 11.041 | 1.00 23.22 | | H | С |
| | | 1698 | | | | -10.765 | 17.696 | 16.007 | | | | |
| | ATOM | | N | VAL H | | | | | 1.00 43.69 | | | N |
| | MOTA | 1699 | ca | VAL H | | -10.733 | 17.251 | 17.385 | 1.00 41.35 | ; | H | C |
| | ATOM | 1700 | С | VAL H | 5 5 | -11.037 | 15.772 | 17.453 | 1.00 38.94 | | H | C |
| | ATOM | 1701 | 0 | VAL H | 5 | -12.140 | 15.350 | 17.142 | 1.00 42.95 | | H | 0 |
| 50 | | | | | 5 | | | | | | | |
| 50 | MOTA | 1702 | CB | VAL H | | -11.757 | 18.027 | 18.225 | 1.00 37.98 | | H | C |
| | ATOM | 1703 | CG1 | VAL H | 5 | -11.835 | 17.437 | 19.607 | 1.00 40.24 | | H | С |
| | MOTA | 1704 | CG2 | VAL H | 5 | -11.357 | 19.487 | 18.296 | 1.00 32.84 | | | C |
| | ATOM | 1705 | N | GLU H | | -10.044 | 14.987 | 17.842 | 1.00 38.45 | | | |
| | | | | | | | | | | | | N |
| | MOTA | 1706 | $^{\rm CA}$ | GLU H | 6 | -10.251 | 13.552 | 18.025 | 1.00 43.30 | | H | C |
| 55 | MOTA | 1707 | С | GLU H | 6 | -10.849 | 13.238 | 19.398 | 1.00 47.18 | | H | С |
| | MOTA | 1708 | 0 | GLU H | | -11.081 | 14.111 | 20.225 | 1.00 53.60 | | | Ō |
| | | | | | | | | | | | | |
| | MOTA | 1709 | CB | GLU H | | -8.899 | 12.855 | 17.872 | 1.00 38.50 | | H | С |
| | MOTA | 1710 | CG | GLU H | 6 | -8.397 | 12.874 | 16.428 | 1.00 34.54 | | H | C |
| | MOTA | 1711 | CD | GLU H | | -7.318 | 13.922 | 16.284 | 1.00 28.64 | | | C |
| 60 | ATOM | 1712 | | GLU H | | -6.427 | 13.847 | 15.454 | 1.00 39.15 | | | Ö |
| | | | | | | | | | | | | |
| | MOTA | 1713 | OE2 | | | -7.420 | 14.934 | 17.168 | 1.00 29.23 | | | 0 |
| | MOTA | 1714 | N | SER H | 7 | -11.141 | 11.940 | 19.613 | 1.00 51.21 |] | H | N |
| | ATOM | 1715 | CA | SER H | | -11.734 | 11.542 | 20.886 | 1.00 53.01 | | | C |
| | | | | | | | | | | | | |
| 05 | ATOM | 1716 | , C | SER H | | -12.123 | 10.061 | 20.902 | 1.00 53.06 | | | C |
| 65 | MOTA | 1717 | 0 | SER H | | -12.030 | 9.347 | 19.912 | 1.00 44.63 |] | H | 0 |
| | MOTA | 1718 | CB | SER H | 7 | -12.975 | 12.403 | 21.122 | 1.00 54.35 | 1 | | С |
| | MOTA | 1719 | ŌĠ | SER H | | -13.927 | 12.149 | 20.088 | 1.00 45.65 | | | ŏ |
| | | | | | | | | | | | | |
| | MOTA | 1720 | N | GLY H | | -12.533 | 9.597 | 22.098 | 1.00 55.02 | | | N |
| | ATOM | 1721 | ca | GLY H | 8 | -12.996 | 8.217 | 22.227 | 1.00 56.76 |] | H | С |
| | | | | | | | | | | | | |

| | ATOM | 1722 | С | GLY H | 8 | -11.834 | 7.227 | 22.355 | 1.00 53.98 | F | I C |
|-----|--------|------|-------------|--------|------|---------|--------|--------|------------|-----|-----|
| | ATOM | 1723 | 0 | GLY H | 8 | -11.927 | 6.062 | 21.992 | 1.00 55.04 | H | |
| | ATOM | 1724 | N | GLY H | 9 | -10.697 | 7.741 | 22.861 | 1.00 48.90 | H | - |
| | ATOM | 1725 | CA | GLY H | 9 | -9.519 | 6.888 | 22.992 | 1.00 49.84 | | |
| p== | | | | | | | | | | H | |
| 5 | ATOM | 1726 | C | GLY H | 9 | -9.206 | 6.567 | 24.456 | 1.00 53.72 | F | |
| | ATOM | 1727 | 0 | GLY H | 9 | -9.129 | 7.434 | 25.316 | 1.00 60.05 | F | I 0 |
| | ATOM | 1728 | N | GLY H | 10 | -9.060 | 5.256 | 24.731 | 1.00 47.72 | H | I N |
| | ATOM | 1729 | CA | GLY H | 10 | -8.739 | 4.834 | 26.090 | 1.00 52.62 | F | |
| | | 1730 | | GLY H | 10 | | 3.502 | | | | |
| | ATOM | | C | | | -7.985 | | 26.101 | 1.00 53.34 | Η | _ |
| 10 | MOTA | 1731 | 0 | GLY H | 10 | -7.434 | 3.054 | 25.105 | 1.00 53.79 | H | O I |
| | ATOM | 1732 | N | LEU H | 11 | -7.938 | 2.883 | 27.295 | 1.00 51.02 | H | I N |
| | ATOM | 1733 | CA | LEU H | 11 | -7.249 | 1.610 | 27.428 | 1.00 42.34 | H | |
| | ATOM | 1734 | C | LEU H | 11 | -8.119 | 0.453 | 26.940 | 1.00 43.65 | H | |
| | | | | | | | | | | | |
| | ATOM | 1735 | 0 | LEU H | 11 | -9.337 | 0.448 | 27.066 | 1.00 44.21 | H | |
| 15 | ATOM | 1736 | CB | LEU H | 11 | -6.895 | 1.413 | 28.903 | 1.00 50.20 | H | I C |
| | ATOM | 1737 | CG | LEU H | 11 | -6.087 | 0.137 | 29.144 | 1.00 36.24 | H | I C |
| | ATOM | 1738 | CD1 | LEU H | 11 | -4.725 | 0.166 | 28.443 | 1.00 43.75 | H | |
| | ATOM | 1739 | | LEU H | 11 | -5.801 | -0.113 | 30.625 | 1.00 59.31 | H | |
| | | 1740 | | | 12 | | -0.533 | | | | |
| | ATOM | | N | VAL H | | -7.453 | | 26.324 | 1.00 42.94 | H | |
| 20 | ATOM | 1741 | CA | VAL H | 12 | -8.179 | -1.712 | 25.883 | 1.00 43.16 | H | |
| | ATOM | 1742 | С | VAL H | 12 | -7.340 | -2.973 | 26.063 | 1.00 47.66 | F | I C |
| | ATOM | 1743 | 0 | VAL H | 12 | -6.127 | -2.931 | 26.226 | 1.00 57.83 | H | |
| | ATOM | 1744 | CB | VAL H | 12 | -8.535 | -1.535 | 24.407 | 1.00 40.29 | H | |
| | | | | | | | | | | | |
| | ATOM | 1745 | | VAL H | 12 | -9.134 | -2.832 | 23.862 | 1.00 46.80 | H | |
| 25 | MOTA | 1746 | CG2 | VAL H | 12 | -9.542 | -0.414 | 24.245 | 1.00 49.39 | H | I C |
| | ATOM | 1747 | N | LYS H | 13 | -8.035 | -4.121 | 26.078 | 1.00 45.71 | H | I N |
| | ATOM | 1748 | CA | LYS H | 13 | -7.316 | -5.381 | 26.174 | 1.00 43.89 | н | |
| | ATOM | 1749 | C | LYS H | 13 | -7.121 | -6.008 | 24.793 | 1.00 40.39 | H | |
| • | _ | 1750 | | LYS H | 13 | | | | | | |
| 00 | ATOM | | 0 | | | -7.975 | -5.934 | 23.920 | 1.00 46.98 | H | |
| 30 | MOTA | 1751 | CB | LYS H | 13 | -8.117 | -6.324 | 27.071 | 1.00 45.28 | H | |
| | ATOM | 1752 | CG | LYS H | 13 | -7.818 | -6.100 | 28.554 | 1.00 67.37 | IH. | r C |
| | ATOM | 1753 | CD | LYS H | 13 | -8.511 | -4.851 | 29.102 | 1.00 88.33 | H | |
| | ATOM | 1754 | CE | LYS H | 13 | -7.655 | -4.105 | 30.133 | 1.00 80.99 | H | |
| | ATOM | 1755 | NZ | LYS H | 13 | -6.458 | -3.569 | 29.486 | 1.00 58.40 | | |
| 05 | | | | | | | | | | H | |
| 35 | MOTA | 1756 | N | PRO H | 14 | -5.976 | -6.651 | 24.544 | 1.00 38.88 | H | |
| | ATOM | 1757 | ca | PRO H | 14 | -5.784 | -7.265 | 23.231 | 1.00 38.32 | H | ı c |
| | MOTA | 1758 | C | PRO H | 14 | -6.971 | -8.123 | 22.837 | 1.00 44.46 | H | |
| | ATOM | 1759 | Õ | PRO H | 14 | -7.434 | -8.952 | 23.617 | 1.00 52.99 | H | |
| | ATOM | 1760 | СВ | PRO H | 14 | -4.496 | -8.076 | 23.401 | 1.00 37.38 | | |
| 40 | | | | | | | | | | H | |
| 40 | MOTA | 1761 | CG | PRO H | 14 | -4.370 | -8.249 | 24.877 | 1.00 40.42 | H | |
| | ATOM | 1762 | $^{\rm CD}$ | PRO H | 14 | -4.849 | -6.948 | 25.435 | 1.00 35.01 | H | I C |
| | MOTA | 1763 | N | GLY H | 15 | -7.466 | -7.903 | 21.624 | 1.00 45.67 | H | Į N |
| | ATOM | 1764 | CA | GLY H | 15 | -8.601 | -8.653 | 21.119 | 1.00 39.69 | Н | |
| | ATOM | 1765 | C | GLY H | 15 | -9.828 | -7.770 | 21.103 | 1.00 42.73 | H | |
| 45 | | 1766 | | GLY H | | -10.789 | | | | | |
| 45 | ATOM | | 0 | | 15 | | -8.044 | 20.389 | 1.00 43.42 | H | |
| | MOTA | 1767 | N | GLY H | 16 | -9.782 | -6.688 | 21.875 | 1.00 44.16 | H | |
| | MOTA | 1768 | ca | GLY H | 16 | -10.913 | -5.781 | 21.952 | 1.00 43.39 | H | I C |
| | ATOM | 1769 | C | GLY H | 16 | -11.219 | -4.862 | 20.775 | 1.00 45.04 | H | C C |
| | MOTA | 1770 | 0 | GLY H | 16 | -10.566 | -4.890 | 19.721 | 1.00 34.85 | Н | |
| 50 | ATOM | 1771 | N | SER H | 17 | -12.238 | -4.030 | 20.986 | 1.00 45.85 | | |
| 30 | | | | | | | | | | H | |
| | MOTA | 1772 | CA | SER H | 17 | -12.700 | -3.076 | 19.994 | 1.00 44.23 | H | |
| | ATOM | 1773 | С | SER H | 17 | -12.735 | -1.670 | 20.566 | 1.00 42.88 | H | t C |
| | MOTA | 1774 | 0 | SER H | 17 | -12.910 | -1.477 | 21.762 | 1.00 43.45 | H | 0 1 |
| | ATOM | 1775 | CB | SER H | 17 | -14.090 | -3.463 | 19.513 | 1.00 44.97 | Н | |
| 55 | ATOM | 1776 | OG | SER H | 17 | -14.056 | -4.768 | 18.969 | 1.00 64.66 | H | |
| 55 | | | | | | | | | | | |
| | MOTA | 1777 | N | LEU H | 18 | -12.582 | -0.690 | 19.688 | 1.00 43.61 | H | |
| | ATOM | 1778 | ca | LEU H | 18 | -12.573 | 0.704 | 20.084 | 1.00 42.03 | H | C |
| | ATOM | 1779 | С | LEU H | 18 | -13.007 | 1.516 | 18.861 | 1.00 39.52 | H | |
| | ATOM | 1780 | Ō | LEU H | 18 | -12.778 | 1.094 | 17.721 | 1.00 39.63 | Н | |
| 60 | | | | | | | | | | | |
| 60 | ATOM | 1781 | CB | LEU H | 18 | -11.155 | 1.083 | 20.512 | 1.00 43.41 | H | |
| | MOTA | 1782 | CG | LEU H | 18 | -10.925 | 2.488 | 21.051 | 1.00 42.39 | H | |
| | MOTA | 1783 | CD1 | LEU H | 18 | -11.722 | 2.666 | 22.321 | 1.00 43.36 | H | C |
| | ATOM | 1784 | | LEU H | 18 | -9.449 | 2.701 | 21.308 | 1.00 59.30 | H | |
| | ATOM | 1785 | N | LYS H | 19 | -13.640 | 2.665 | 19.090 | 1.00 36.47 | H | |
| 6E | | | | | | | | | | | |
| 65 | MOTA | 1786 | CA | LYS H | 19 | -13.988 | 3.483 | 17.933 | 1.00 42.76 | H | |
| | MOTA | 1787 | С | LYS H | 19 | -13.744 | 4.971 | 18.198 | 1.00 40.99 | Н | |
| | ATOM | 1788 | 0 | LYS H | 19 | -14.288 | 5.562 | 19.121 | 1.00 42.24 | H | |
| | ATOM | 1789 | СВ | LYS H | 19 | -15.465 | 3.247 | 17.608 | 1.00 43.96 | H | |
| | ATOM | 1790 | CG | LYS H | 19 | -15.854 | 3.803 | 16.236 | 1.00 56.00 | H | |
| | WT OLI | 1120 | CG | TITO U | J. 7 | -10.004 | 5.003 | TO.720 | 4.00 50.00 | н | |

| | MOTA | 1791 | CD | LYS H | 19 | -17.256 | 4.416 | 16.235 | 1.00 45.68 | H | C |
|----|------|--------------|-----|-------|----|---------|--------|--------|------------|----|---|
| | ATOM | 1792 | CE | LYS H | 19 | -18.247 | 3.614 | 15.384 | 1.00 59.48 | H | C |
| | MOTA | 1793 | NZ | LYS H | 19 | -19.100 | 4.529 | 14.629 | 1.00 51.55 | H | N |
| | ATOM | 1794 | N | LEU H | 20 | -13.082 | 5.326 | 17.249 | 1.00 39.79 | H | N |
| 5 | ATOM | 1795 | CA | LEU H | 20 | -12.538 | 6.662 | 17.450 | 1.00 36.68 | H | C |
| 5 | | | | | | | | | 1.00 34.74 | | |
| | ATOM | 1796 | C | LEU H | 20 | -13.376 | 7.653 | 16.679 | | H | Č |
| | ATOM | 1797 | 0 | LEU H | 20 | -14.020 | 7.303 | 15.694 | 1.00 33.37 | H | 0 |
| | MOTA | 1798 | CB | LEU H | 20 | -11.096 | 6.779 | 16.945 | 1.00 40.64 | H | С |
| | ATOM | 1799 | CG | LEU H | 20 | -9.905 | 6.022 | 17.535 | 1.00 41.11 | H | C |
| 10 | MOTA | 1800 | | LEU H | 20 | -8.614 | 6.271 | 16.759 | 1.00 61.71 | H | C |
| 10 | ATOM | 1801 | | LEU H | 20 | -9.778 | 6.454 | 18.977 | 1.00 35.59 | H | č |
| | / | | | | | | | | | | |
| | MOTA | 1802 | N | SER H | 21 | -13.497 | 9.005 | 16.927 | 1.00 33.19 | H | N |
| | MOTA | 1803 | CA | SER H | 21 | -14.281 | 9.919 | 16.122 | 1.00 40.56 | H | C |
| | ATOM | 1804 | С | SER H | 21 | -13.489 | 11.202 | 15.983 | 1.00 42.41 | H | C |
| 15 | ATOM | 1805 | 0 | SER H | 21 | -12.563 | 11.461 | 16.753 | 1.00 44.66 | H | 0 |
| | MOTA | 1806 | CB | SER H | 21 | -15.634 | 10.204 | 16.768 | 1.00 34.42 | H | C |
| | ATOM | 1807 | ŌĠ | SER H | 21 | -15.449 | 10.839 | 18.008 | 1.00 46.92 | H | ŏ |
| | ATOM | 1808 | N | CYS H | 22 | -13.846 | 11.997 | 14.988 | 1.00 37.06 | H | |
| | | | | | | | | | | | N |
| | MOTA | 1809 | CA | CYS H | 22 | -13.155 | 13.242 | 14.739 | 1.00 38.14 | H | C |
| 20 | ATOM | 1810 | C | CYS H | 22 | -14.158 | 14.285 | 14.346 | 1.00 31.54 | H | C |
| | MOTA | 1811 | 0 | CYS H | 22 | -14.810 | 14.172 | 13.318 | 1.00 30.64 | H | 0 |
| | ATOM | 1812 | CB | CYS H | 22 | -12.135 | 13.057 | 13.612 | 1.00 43.73 | H | C |
| | MOTA | 1813 | SG | CYS H | 22 | -11.198 | 14.513 | 13.004 | 1.00 55.55 | H | S |
| | MOTA | 1814 | N | ALA H | 23 | -14.284 | 15.298 | 15.190 | 1.00 32.03 | H | N |
| 25 | | 1815 | | ALA H | 23 | -15.187 | 16.402 | 14.926 | 1.00 32.05 | H | |
| 25 | ATOM | | CA | | | | | | | | C |
| | MOTA | 1816 | C | ALA H | 23 | -14.445 | 17.364 | 14.002 | 1.00 39.56 | H | C |
| | ATOM | 1817 | 0 | ALA H | 23 | -13.378 | 17.893 | 14.348 | 1.00 37.69 | H | 0 |
| | MOTA | 1818 | CB | ALA H | 23 | -15.552 | 17.089 | 16.220 | 1.00 38.17 | H | С |
| | ATOM | 1819 | N | ALA H | 24 | -14.992 | 17.572 | 12.814 | 1.00 36.81 | H | N |
| 30 | MOTA | 1820 | CA | ALA H | 24 | -14.362 | 18.465 | 11.867 | 1.00 31.76 | H | C |
| 00 | ATOM | 1821 | C | ALA H | 24 | ~15.091 | 19.800 | 11.857 | 1.00 34.30 | H | č |
| | | | | | 24 | -16.200 | 19.910 | 12.368 | 1.00 34.50 | | |
| | MOTA | 1822 | 0 | ALA H | | | | | | H | 0 |
| | MOTA | 1823 | CB | ALA H | 24 | -14.379 | 17.836 | 10.481 | 1.00 29.25 | H | С |
| | MOTA | 1824 | N | SER H | 25 | -14.456 | 20.811 | 11.275 | 1.00 45.22 | H | N |
| 35 | MOTA | 1825 | CA | SER H | 25 | -15.040 | 22.146 | 11.173 | 1.00 45.48 | H | C |
| | ATOM | 1826 | C | SER H | 25 | -14.022 | 23.142 | 10.638 | 1.00 45.04 | H | C |
| | MOTA | 1827 | Ō | SER H | 25 | -12.823 | 22.995 | 10.862 | 1.00 48.34 | H | Ó |
| | ATOM | 1828 | ČВ | SER H | 25 | -15.509 | 22.637 | 12.535 | 1.00 45.05 | H | č |
| | | | | | | | | | | | |
| 40 | ATOM | 1829 | OG | SER H | 25 | -14.401 | 22.994 | 13.327 | 1.00 38.97 | H | 0 |
| 40 | ATOM | 1830 | N | GLY H | 26 | -14.510 | 24.163 | 9.943 | 1.00 43.04 | H | M |
| | ATOM | 1831 | CA | GLY H | 26 | -13.627 | 25.181 | 9.417 | 1.00 36.80 | H | C |
| | MOTA | 1832 | C | GLY H | 26 | -13.361 | 24.980 | 7.951 | 1.00 38.49 | H | C |
| | MOTA | 1833 | 0 | GLY H | 26 | -12.549 | 25.684 | 7.362 | 1.00 52.85 | H | 0 |
| | MOTA | 1834 | N | PHE H | 27 | -14.035 | 24.007 | 7.356 | 1.00 37.93 | Ħ | N |
| 45 | ATOM | 1835 | CA | PHE H | 27 | -13.856 | 23.745 | 5.946 | 1.00 34.05 | H | C |
| .0 | MOTA | 1836 | C | PHE H | 27 | -15.015 | 22.930 | 5.427 | 1.00 36.91 | H | Č |
| | | | | | | -15.759 | 22.343 | | | | |
| | ATOM | 1837 | 0 | PHE H | 27 | | | 6.206 | 1.00 39.00 | H | 0 |
| | MOTA | 1838 | CB | PHE H | 27 | ~12.522 | 23.017 | 5.670 | 1.00 33.34 | H | C |
| | MOTA | 1839 | CG | PHE H | 27 | -12.394 | 21.675 | 6.329 | 1.00 17.41 | H | C |
| 50 | MOTA | 1840 | CD1 | PHE H | 27 | -12.133 | 21.570 | 7.691 | 1.00 25.29 | H | C |
| | MOTA | 1841 | CD2 | PHE H | 27 | -12.547 | 20.512 | 5.586 | 1.00 15.22 | H | C |
| | MOTA | 1842 | CE1 | | 27 | -12.030 | 20.319 | 8.304 | 1.00 21.74 | H | C |
| | ATOM | 1843 | CE2 | | 27 | -12.447 | 19.265 | 6.188 | 1.00 8.67 | H | Ċ |
| | | 1844 | CZ | PHE H | 27 | -12.188 | 19.167 | 7.547 | 1.00 16.97 | | Č |
| | ATOM | | | | | | | | | H | |
| 55 | MOTA | 1845 | N | THR H | 28 | -15.168 | 22.907 | 4.108 | 1.00 38.20 | H | N |
| | MOTA | 1846 | CA | THR H | 28 | -16.238 | 22.176 | 3.457 | 1.00 35.35 | H | C |
| | MOTA | 1847 | C | THR H | 28 | -15.956 | 20.675 | 3.520 | 1.00 35.62 | H | C |
| | MOTA | 1848 | 0 | THR H | 28 | -15.657 | 20.042 | 2.510 | 1.00 41.35 | H | 0 |
| | MOTA | 1849 | CB | THR H | 28 | -16.349 | 22.645 | 2.007 | 1.00 37.46 | H | C |
| 60 | MOTA | 1850 | OG1 | | 28 | -16.428 | 24.074 | 1.989 | 1.00 41.29 | Н | Ō |
| 00 | MOTA | 1851 | CG2 | THR H | 28 | -17.575 | 22.066 | 1.340 | 1.00 44.03 | H | č |
| | | | | | | | | | | | |
| | MOTA | 1852 | N | PHE H | 29 | -16.063 | 20.130 | 4.728 | 1.00 34.25 | H | N |
| | MOTA | 1853 | CA | PHE H | 29 | -15.818 | 18.721 | 5.042 | 1.00 34.22 | H | C |
| | MOTA | 1854 | C | PHE H | 29 | -16.163 | 17.674 | 3.979 | 1.00 34.25 | H | C |
| 65 | ATOM | 1855 | 0 | PHE H | 29 | -15.391 | 16.755 | 3.730 | 1.00 47.37 | H | 0 |
| | MOTA | 1856 | CB | PHE H | 29 | -16.530 | 18.390 | 6.356 | 1.00 33.13 | H | C |
| | ATOM | 1857 | CG | PHE H | 29 | -16.417 | 16.954 | 6.771 | 1.00 30.33 | H | Ċ |
| | MOTA | 1858 | | PHE H | 29 | -17.427 | 16.055 | 6.481 | 1.00 33.76 | H | Č |
| | | 1859 | | PHE H | 29 | -15.298 | 16.505 | 7.462 | 1.00 38.72 | H | C |
| | MOTA | TOJ 2 | CDZ | CHE D | 43 | -13.270 | 70.202 | 1.404 | 1.00 20.74 | 11 | |

| | | | | | _ | | | | | | |
|-----|------|------|-------|------|----|---------|--------|--------|------------|---|----|
| | MOTA | 1860 | CE1 P | | 29 | -17.325 | 14.740 | 6.872 | 1.00 41.24 | H | С |
| | MOTA | 1861 | | HE H | 29 | -15.189 | 15.193 | 7.855 | 1.00 25.21 | H | C |
| | MOTA | 1862 | | HE H | 29 | -16.205 | 14.307 | 7.560 | 1.00 31.25 | H | C |
| | MOTA | 1863 | | LE H | 30 | -17.316 | 17.813 | 3.347 | 1.00 35.57 | H | N |
| 5 | MOTA | 1864 | | LE H | 30 | -17.752 | 16.875 | 2.324 | 1.00 36.50 | H | C |
| | ATOM | 1865 | C I | LE H | 30 | -16.860 | 16.824 | 1.080 | 1.00 38.95 | H | C |
| | MOTA | 1866 | O I: | LE H | 30 | -16.809 | 15.809 | 0.376 | 1.00 40.39 | H | 0 |
| | MOTA | 1867 | CB I | LE H | 30 | -19.182 | 17.220 | 1.867 | 1.00 36.84 | H | С |
| | MOTA | 1868 | CG1 I | LE H | 30 | -19.637 | 16.259 | 0.770 | 1.00 35.17 | H | C |
| 10 | ATOM | 1869 | CG2 I | LE H | 30 | -19.225 | 18.663 | 1.356 | 1.00 36.84 | H | C |
| | ATOM | 1870 | | LE H | 30 | -21.038 | 16.515 | 0.308 | 1.00 43.88 | H | Č |
| | ATOM | 1871 | - | ER H | 31 | -16.153 | 17.907 | 0.795 | 1.00 33.28 | H | N |
| | ATOM | 1872 | | ER H | 31 | -15.332 | 17.915 | -0.403 | 1.00 37.16 | H | C |
| | ATOM | 1873 | | ER H | 31 | -13.914 | 17.386 | -0.236 | 1.00 38.76 | H | Č |
| 15 | ATOM | 1874 | | ER H | 31 | -13.159 | 17.306 | -1.208 | 1.00 39.05 | н | Õ |
| 10 | ATOM | 1875 | | ER H | 31 | -15.304 | 19.319 | -1.010 | 1.00 33.72 | H | č |
| | ATOM | 1876 | | ER H | 31 | -16.600 | 19.717 | -1.417 | 1.00 41.28 | H | ŏ |
| | ATOM | 1877 | | YR H | 32 | -13.570 | 17.001 | 0.988 | 1.00 37.10 | H | N |
| | ATOM | 1878 | | YR H | 32 | -12.240 | 16.483 | 1.273 | 1.00 37.10 | H | C |
| 20 | MOTA | 1879 | | YR H | 32 | -12.172 | 14.998 | 1.621 | 1.00 35.75 | H | C |
| 20 | ATOM | 1880 | | YR H | 32 | -13.125 | 14.414 | 2.126 | 1.00 35.73 | H | Ö |
| | ATOM | 1881 | | YR H | 32 | -11.622 | 17.265 | 2.419 | 1.00 33.07 | н | c |
| | | 1882 | | YR H | 32 | -11.220 | 18.657 | 2.056 | 1.00 31.67 | | |
| | ATOM | | | | | | | | | H | C |
| 05 | MOTA | 1883 | | YR H | 32 | -10.063 | 18.895 | 1.343 | 1.00 40.11 | H | C |
| 25 | ATOM | 1884 | _ | YR H | 32 | -11.997 | 19.735 | 2.418 | 1.00 27.93 | H | C |
| | ATOM | 1885 | | YR H | 32 | -9.692 | 20.165 | 0.998 | 1.00 30.26 | H | C |
| | ATOM | 1886 | | YR H | 32 | -11.633 | 21.001 | 2.082 | 1.00 43.25 | H | C |
| | ATOM | 1887 | | YR H | 32 | -10.475 | 21.214 | 1.368 | 1.00 39.71 | H | C |
| | ATOM | 1888 | | YR H | 32 | -10.103 | 22.493 | 1.026 | 1.00 65.73 | H | 0 |
| 30 | MOTA | 1889 | | LA H | 33 | -11.024 | 14.399 | 1.326 | 1.00 33.25 | H | N |
| | MOTA | 1890 | | LA H | 33 | -10.781 | 13.010 | 1.657 | 1.00 35.61 | Н | Ç |
| | MOTA | 1891 | | LA H | 33 | -10.282 | 13.125 | 3.084 | 1.00 36.27 | H | C. |
| | ATOM | 1892 | | LA H | 33 | -9.672 | 14.131 | 3.446 | 1.00 31.77 | H | 0 |
| | MOTA | 1893 | CB A | LA H | 33 | -9.707 | 12.433 | 0.779 | 1.00 28.41 | H | C |
| 35 | MOTA | 1894 | | ET H | 34 | -10.556 | 12.116 | 3.899 | 1.00 33.27 | H | N |
| | MOTA | 1895 | CA M | ET H | 34 | -10.120 | 12.147 | 5.283 | 1.00 28.49 | H | C |
| | MOTA | 1896 | C M | ET H | 34 | -9.231 | 10.958 | 5.555 | 1.00 28.00 | H | C |
| | MOTA | 1897 | O M | ET H | 34 | -9.373 | 9.917 | 4.921 | 1.00 27.81 | H | 0 |
| | MOTA | 1898 | CB M | ET H | 34 | -11.324 | 12.147 | 6.226 | 1.00 31.24 | H | С |
| 40 | MOTA | 1899 | CG M | ET H | 34 | -12.122 | 13.436 | 6.180 | 1.00 30.32 | H | С |
| | MOTA | 1900 | SD M | ET H | 34 | -11.099 | 14.933 | 6.419 | 1.00 39.20 | H | S |
| | MOTA | 1901 | CE M | ET H | 34 | -10.854 | 14.939 | 8.175 | 1.00 17.55 | H | С |
| | MOTA | 1902 | N S | ER H | 35 | -8.308 | 11.113 | 6.497 | 1.00 28.90 | H | N |
| | MOTA | 1903 | CA S | ER H | 35 | -7.391 | 10.035 | 6.808 | 1.00 24.89 | H | С |
| 45 | MOTA | 1904 | C S | ER H | 35 | -7.009 | 9.890 | 8.265 | 1.00 33.44 | H | С |
| | ATOM | 1905 | o s | ER H | 35 | -7.102 | 10.828 | 9.045 | 1.00 35.02 | H | 0 |
| | MOTA | 1906 | CB S | ER H | 35 | -6.118 | 10.200 | 5.990 | 1.00 21.68 | H | C |
| | MOTA | 1907 | og s | ER H | 35 | -6.378 | 10.012 | 4.612 | 1.00 32.05 | H | 0 |
| | MOTA | 1908 | N T | RP H | 36 | -6.591 | 8.686 | 8.631 | 1.00 34.43 | H | N |
| 50 | MOTA | 1909 | CA T | RP H | 36 | -6.130 | 8.441 | 9.980 | 1.00 31.01 | H | С |
| | MOTA | 1910 | C T | RP H | 36 | -4.651 | 8.041 | 9.863 | 1.00 33.80 | H | C |
| | ATOM | 1911 | | RP H | 36 | -4.286 | 7.210 | 9.029 | 1.00 38.52 | H | 0 |
| | ATOM | 1912 | | RP H | 36 | -6.945 | 7.324 | 10.643 | 1.00 30.03 | H | C |
| | ATOM | 1913 | | RP H | 36 | -8.340 | 7.724 | 11.080 | 1.00 24.72 | H | Č |
| 55 | ATOM | 1914 | | RP H | 36 | -9.498 | 7.546 | 10.386 | 1.00 25.13 | H | Č |
| 00 | MOTA | 1915 | | RP H | 36 | -8.710 | 8.348 | 12.319 | 1.00 27.37 | H | Č |
| | ATOM | 1916 | | RP H | 36 | -10.565 | 8.016 | 11.112 | 1.00 29.30 | H | N |
| | ATOM | 1917 | | RP H | 36 | -10.109 | 8.512 | 12.303 | 1.00 25.16 | H | Ĉ |
| | ATOM | 1918 | | RP H | 36 | -7.994 | 8.780 | 13.443 | 1.00 32.09 | H | C |
| 60 | ATOM | 1919 | | RP H | 36 | -10.809 | 9.089 | 13.365 | 1.00 32.03 | H | C |
| 00 | | 1920 | | | 36 | -8.687 | 9.355 | 14.501 | 1.00 22.13 | H | ~ |
| | MOTA | 1920 | | RP H | | | 9.502 | | | | C |
| | MOTA | 1921 | | RP H | 36 | -10.081 | | 14.454 | 1.00 18.64 | H | C |
| | ATOM | 1922 | | AL H | 37 | -3.802 | 8.664 | 10.670 | 1.00 28.90 | H | N |
| GE. | MOTA | 1923 | | AL H | 37 | -2.369 | 8.367 | 10.672 | 1.00 28.13 | H | C |
| 65 | ATOM | 1924 | | AL H | 37 | -1.922 | 8.214 | 12.115 | 1.00 27.45 | H | С |
| | ATOM | 1925 | | AL H | 37 | -2.258 | 9.032 | 12.968 | 1.00 32.69 | H | 0 |
| | ATOM | 1926 | | AL H | 37 | -1.537 | 9.507 | 10.052 | 1.00 23.26 | H | C |
| | ATOM | 1927 | CG1 V | | 37 | -0.087 | 9.102 | 9.998 | 1.00 29.09 | H | C |
| | ATOM | 1928 | CG2 V | аь Н | 37 | -2.043 | 9.846 | 8.670 | 1.00 31.03 | H | C |

| | MOT:A | 1929 | N | ARG H | 3 8 | -1.164 | 7.178 | 12.414 | 1.00 26.98 | H | N |
|----|--------------|--------------|------------|----------------|---------------|------------------|------------------|------------------|--------------------------|--------|--------|
| | MOTA | 1930 | CA | ARG H | 38 | -0.736 | 7.018 | 13.796 | 1.00 31.26 | H | Ċ |
| | MOTA | 1931 | С | ARG H | 38 | 0.766 | 7.128 | 13.979 | 1.00 34.92 | H | С |
| | MOTA | 1932 | 0 | ARG H | 38 | 1.539 | 7.100 | 13.011 | 1.00 36.42 | H | 0 |
| 5 | ATOM | 1933 | CB | ARG H | 38 | -1.218 | 5.685 | 14.357 | 1.00 30.82 | H | С |
| | MOTA | 1934 | CG | ARG H | 38 | -0.548 | 4.505 | 13.732 | 1.00 32.29 | H | С |
| | ATOM | 1935 | CD | ARG H | 38 | -1.297 | 3.253 | 14.078 | 1.00 31.61 | H | C |
| | MOTA MOTA | 1936 1937 | NE | ARG H | 38 38 | -0.684 | 2.082 0.855 | 13.471 13.568 | 1.00 45.30 1.00 49.14 | H | N |
| 10 | MOTA | 1938 | CZ | ARG H ARG H | 38 | -1.174 -2.288 | 0.833 | 14.256 | 1.00 49.14 | H H | C N |
| 10 | ATOM | 1939 | | ARG H | 38 | -0.556 | -0.155 | 12.971 | 1.00 39.29 | H | N |
| | MOTA | 1940 | N | GLN H | 39 | 1.161 | 7.297 | 15.237 | 1.00 34.35 | H | N |
| | MOTA | 1941 | CA | GLN H | 39 | 2.564 | 7.394 | 15.600 | 1.00 36.21 | H | Ĉ |
| | ATOM | 1942 | С | GLN H | 39 | 2.768 | 6.396 | 16.714 | 1.00 32.94 | H | Č |
| 15 | MOTA | 1943 | 0 | GLN H | 39 | 2.097 | 6.442 | 17.739 | 1.00 36.86 | H | 0 |
| | MOTA | 1944 | СВ | GLN H | 39 | 2.902 | 8.804 | 16.073 | 1.00 35.48 | H | C |
| | MOTA | 1945 | CG | GLN H | 39 | 4.375 | 9.038 | 16.273 | 1.00 40.46 | H | C |
| | MOTA | 1946 | CD CE1 | GLN H | 39 | 4.718 | 10.507 | 16.381 | 1.00 30.97 | H | C |
| 20 | ATOM ATOM | 1947 1948 | OE1 NE2 | | 39 39 | 4.023 5.798 | 11.276 10.903 | 17.039 15.742 | 1.00 46.87 | H | O |
| 20 | ATOM | 1948 | NEZ N | THR H | 40 | 3.681 | 5.468 | 16.498 | 1.00 39.13 1.00 32.21 | H H | N |
| | MOTA | 1950 | CA | THR H | 40 | 3.951 | 4.444 | 17.485 | 1.00 32.21 | H | _ C |
| | ATOM | 1951 | C | THR H | 40 | 4.794 | 5.034 | 18.596 | 1.00 36.27 | H | Č |
| | MOTA | 1952 | 0 | THR H | 40 | 5.338 | 6.131 | 18.466 | 1.00 33.90 | Н | Ō |
| 25 | ATOM | 1953 | CB | THR H | 40 | 4.707 | 3.278 | 16.860 | 1.00 25.60 | H | C |
| | MOTA | 1954 | OG1 | | 40 | 6.056 | 3.676 | 16.592 | 1.00 30.95 | H | 0 |
| | ATOM | 1955 | CG2 | | 40 | 4.049 | 2.867 | 15.552 | 1.00 19.81 | H | C |
| | MOTA | 1956 | N | PRO H | 41 | 4.891 | 4.319 | 19.721 | 1.00 43.34 | H | И |
| 30 | MOTA MOTA | 1957 1958 | CA C | PRO H PRO H | 41 41 | $5.674 \\ 7.119$ | 4.853 5.054 | 20.826 20.383 | 1.00 42.33 1.00 40.47 | H H | C |
| 30 | MOTA | 1959 | Ö | PRO H | 41 | 7.882 | 5.837 | 20.938 | 1.00 46.47 | H | Ö |
| | ATOM | 1960 | ČВ | PRO H | 41 | 5.609 | 3.858 | 21.983 | 1.00 46.00 | H | č |
| | MOTA | 1961 | CG | PRO H | 41 | 4.463 | 2.890 | 21.713 | 1.00 44.54 | H | Č |
| | ATOM | 1962 | CD | PRO H | 41 | 4.124 | 3.171 | 20.174 | 1.00 37.36 | H | C |
| 35 | MOTA | 1963 | N | GLU H | 42 | 7.491 | 4.257 | 19.367 | 1.00 39.84 | H | N |
| | ATOM | 1964 | CA | GLU H | 42 | 8.779 | 4.449 | 18.727 | 1.00 39.67 | H | С |
| | MOTA | 1965 | C | GLU H | 42 | 8.724 | 5.653 | 17.788 | 1.00 39.72 | H | C |
| | MOTA | 1966 | 0 | GLU H | 42 | 9.627 | 5.927 | 17.009 | 1.00 38.24 | H | 0 |
| 40 | MOTA MOTA | 1967 1968 | CB CG | GLU H | 42 42 | 9.119 9.167 | 3.172 1.932 | 17.953 18.853 | 1.00 43.69 1.00 59.11 | H H | C |
| 40 | ATOM | 1969 | CD | GLU H | 42 | 7.786 | 1.324 | 18.945 | 1.00 78.32 | H | C |
| | MOTA | 1970 | | GLU H | 42 | 7.323 | 0.767 | 17.959 | 1.00 71.16 | H | ŏ |
| | ATOM | 1971 | | GLU H | 42 | 7.189 | 1.394 | 20.020 | 1.00 93.36 | Н | ŏ |
| | ATOM | 1972 | N | LYS H | 43 | 7.571 | 6.354 | 17.856 | 1.00 37.86 | H | N |
| 45 | ATOM | 1973 | CA | LYS H | 43 | 7.470 | 7.658 | 17.210 | 1.00 31.78 | H | C |
| | MOTA | 1974 | C | LYS H | 43 | 7.569 | 7.568 | 15.691 | 1.00 30.82 | H | C |
| | ATOM | 1975 | O | LYS H | 43 | 7.922 | 8.523 | 15.010 | 1.00 34.06 | H | 0 |
| | ATOM ATOM | 1976 1977 | CB CG | LYS H LYS H | 43 43 | 8.596 8.330 | 8.534 8.971 | 17.748 19.189 | 1.00 30.63 1.00 45.46 | H H | C |
| 50 | ATOM | 1978 | CD | LYS H | 43 | 9.247 | 10.113 | 19.627 | 1.00 83.82 | H | Č |
| | ATOM | 1979 | CE | LYS H | 43 | 10.474 | 9.615 | 20.395 | 1.00 96.13 | H | Č |
| | ATOM | 1980 | NZ | LYS H | 43 | 10.052 | 9.064 | 21.680 | 1.00 87.58 | H | N |
| | MOTA | 1981 | N | ARG H | 44 | 7.156 | 6.442 | 15.122 | 1.00 29.41 | H | N |
| | ATOM | 1982 | CA | ARG H | 44 | 7.087 | 6.323 | 13.668 | 1.00 29.46 | H | C |
| 55 | ATOM | 1983 | Č | ARG H | 44 | 5.640 | 6.520 | 13.204 | 1.00 33.48 | H | C |
| | ATOM | 1984 | 0 | ARG H | 44 | 4.710 | 5.953 | 13.787 | 1.00 37.98 | H | 0 |
| | ATOM | 1985 1986 | CB | ARG H | 44 | 7.574 | 4.951 4.701 | 13.197 | 1.00 31.50 | H | C |
| | ATOM ATOM | 1987 | CG CD | ARG H ARG H | 44 44 | 9.044 9.456 | 3.351 | 13.379 12.802 | 1.00 35.58 1.00 56.91 | H H | C |
| 60 | MOTA | 1988 | NE | ARG H | 44 | 9.904 | 3.439 | 11.412 | 1.00 71.87 | H | И |
| | ATOM | 1989 | CZ | ARG H | 44 | 10.966 | 4.139 | 11.007 | 1.00 70.52 | H | C |
| | MOTA | 1990 | | ARG H | $\frac{1}{4}$ | 11.989 | 4.322 | 11.832 | 1.00 72.59 | H | Ŋ |
| | ATOM | 1991 | | ARG H | 44 | 10.995 | 4.672 | 9.785 | 1.00 65.12 | H | Ŋ |
| | MOTA | 1992 | N | LEU H | 45 | 5.457 | 7.315 | 12.150 | 1.00 30.81 | H | N |
| 65 | ATOM | 1993 | CA | LEU H | 45 | 4.131 | 7.577 | 11.597 | 1.00 23.62 | H | C |
| | ATOM | 1994 | C | LEU H | 45 | 3.688 | 6.488 | 10.611 | 1.00 28.24 | H | C |
| | ATOM | 1995 | 0 | LEU H | 45 | 4.461 | 6.058 | 9.767 | 1.00 26.20 | H | 0 |
| | MOTA | 1996 | CB | LEU H | 45 | 4.131 | 8.938 | 10.898 | 1.00 18.00 | H | C |
| | MOTA | 1997 | CG | LEU H | 45 | 4.392 | 10.152 | 11.794 | 1.00 19.88 | H | С |

| | ATOM | 1998 | CD1 | LEU H | 45 | 4.867 | 11.310 | 10.938 | 1.00 24.54 | | Н | С |
|----|--------------|--------------|------------|----------------|----------|--------------------|------------------|-------------------|--------------------------|---|--------|---------------|
| | ATOM | 1999 | | | 45 | 3.131 | 10.522 | 12.590 | 1.00 14.97 | | H | C |
| | ATOM ATOM | 2000 2001 | N CA | GLU H GLU H | 46 46 | $2.445 \\ 1.924$ | 6.038 5.022 | 10.725 9.818 | 1.00 28.38 1.00 26.32 | | H H | N C |
| 5 | ATOM | 2001 | C | GLU H | 46 | 0.508 | 5.374 | 9.344 | 1.00 26.58 | | H | Č |
| • | ATOM | 2003 | ō | GLU H | 46 | -0.411 | 5.473 | 10.152 | 1.00 33.14 | | H | 0 |
| | MOTA | 2004 | CB | GLU H | 46 | 1.874 | 3.638 | 10.496 | 1.00 35.21 | • | H | C |
| | MOTA | 2005 | | GLU H | 46 | 2.847 2.785 | 3.393 1.943 | 11.668 12.231 | 1.00 49.18 1.00 64.81 | | H H | C |
| 10 | ATOM ATOM | 2006 2007 | CD OE1 | GLU H | 46 46 | 1.691 | 1.473 | 12.630 | 1.00 67.38 | | H | Ö |
| 10 | ATOM | 2007 | | GLU H | 46 | 3.844 | 1.269 | 12.280 | 1.00 52.21 | | H | ŏ |
| | MOTA | 2009 | N | TRP H | 47 | 0.327 | 5.577 | 8.045 | 1.00 30.57 | | H | N |
| | ATOM | 2010 | CA | TRP H | 47 | -1.012 | 5.751 | 7.500 | 1.00 25.48 | | H | C |
| 45 | MOTA | 2011 | C | TRP H | 47 47 | -1.886 -1.548 | 4.524 3.393 | 7.770 7.443 | 1.00 30.87 1.00 32.26 | | H H | C |
| 15 | ATOM ATOM | 2012 2013 | O CB | TRP H | 47 | -0.885 | 5.991 | 5.996 | 1.00 32.25 | | H | č |
| | ATOM | 2014 | CG | TRP H | 47 | -2.202 | 5.841 | 5.341 | 1.00 23.75 | | H | C |
| | MOTA | 2015 | CD1 | TRP H | 47 | -3.297 | 6.729 | 5.426 | 1.00 36.84 | | H | C |
| | ATOM | 2016 | CD2 | TRP H | 47 | -2.617 | 4.754 | 4.481 | 1.00 23.08 | | H | C |
| 20 | ATOM ATOM | 2017 2018 | NE1 CE2 | TRP H | 47 47 | -4.364 -3.948 | 6.308 5.025 | $4.697 \\ 4.078$ | 1.00 39.41 1.00 27.40 | | H H | C N |
| • | MOTA | 2019 | CE2 | TRP H | 47 | -1.989 | 3.594 | 4.036 | 1.00 23.52 | | H | Č |
| | ATOM | 2020 | CZ2 | TRP H | 47 | -4.609 | 4.142 | 3.240 | 1.00 16.46 | | H | C |
| | MOTA | 2021 | CZ3 | TRP H | 47 | -2.651 | 2.710 | 3.200 | 1.00 22.42 | | H | C |
| 25 | MOTA | 2022 | CH2 | TRP H VAL H | 47 48 | -3.972 -3.034 | $2.986 \\ 4.778$ | 2.803 8.426 | 1.00 27.75 1.00 35.93 | | H H | C N |
| | MOTA ATOM | 2023 2024 | N CA | VAL H | 48 | -3.887 | 3.671 | 8.844 | 1.00 33.96 | | H | C |
| | ATOM | 2025 | C | VAL H | 48 | -5.099 | 3.492 | 7.925 | 1.00 31.29 | | H | C |
| | MOTA | 2026 | 0 | VAL H | 48 | -5.503 | 2.386 | 7.586 | 1.00 34.83 | | H | 0 |
| 30 | MOTA | 2027 | CB | VAL H | 48 | -4.355 | 3.947 | 10.273 | 1.00 31.31 1.00 45.32 | | H H | C |
| | ATOM ATOM | 2028 2029 | | VAL H VAL H | 48 48 | -5.379 -3.171 | 2.896 3.907 | 10.698 11.221 | 1.00 40.07 | | п Н | C |
| | ATOM | 2030 | N | ALA H | 49 | -5.715 | 4.632 | 7.555 | 1.00 32.57 | | H | N |
| | MOTA | 2031 | CA | ALA H | 49 | -6.900 | 4.560 | 6.706 | 1.00 30.97 | | H | C |
| 35 | MOTA | 2032 | C | ALA H | 49 | -7.176 | 5.889 | 5.996 | 1.00 31.41 | | H | C |
| | MOTA | 2033 | O | ALA H ALA H | 49 49 | -6.710 -8.093 | $6.947 \\ 4.181$ | 6.399 7.585 | 1.00 35.89 1.00 27.71 | | H H | C |
| | MOTA MOTA | 2034 2035 | CB N | SER H | 50 | -7.942 | 5.801 | 4.915 | 1.00 28.70 | | H | N |
| | ATOM | 2036 | CA | SER H | 50 | -8.289 | 6.962 | 4.113 | 1.00 31.27 | | H | C |
| 40 | MOTA | 2037 | С | SER H | 50 | -9.629 | 6.737 | 3.442 | 1.00 33.01 | | H | C |
| | ATOM | 2038 | 0 | SER H | 50 | -9.863 | 5.703 | 2.820 | 1.00 33.77 | | H H | C |
| | MOTA MOTA | 2039 2040 | CB OG | SER H SER H | 50 50 | -7.229 -6.021 | 7.220 7.678 | 3.036 3.604 | 1.00 29.77 1.00 36.87 | | H | Ö |
| | ATOM | 2040 | И | ILE H | 51 | -10.508 | 7.717 | 3.575 | 1.00 31.73 | | H | N |
| 45 | MOTA | 2042 | CA | ILE H | 51 | -11.828 | 7.646 | 2.978 | 1.00 30.25 | | H | C |
| | MOTA | 2043 | C | ILE H | 51 | -11.958 | 8.838 | 2.032 | 1.00 33.02 | | H | C |
| | MOTA | 2044 2045 | O CB | ILE H | 51 51 | -11.591 -12.919 | 9.966 7.695 | 2.380 4.079 | 1.00 35.69 1.00 29.54 | | H H | 0 |
| | MOTA MOTA | 2045 | CG1 | | 51 | -14.287 | 7.379 | 3.479 | 1.00 26.92 | | H | Č |
| 50 | ATOM | 2047 | CG2 | | 51 | -12.925 | 9.051 | 4.754 | 1.00 23.38 | 3 | H | C |
| | ATOM | 2048 | | ILE H | 51 | -15.356 | 7.192 | 4.510 | 1.00 38.16 | | H | C |
| | ATOM | 2049 2050 | N CA | SER H SER H | 52 52 | -12.450 -12.533 | 8.600 9.725 | 0.828 -0.096 | 1.00 32.29 1.00 37.72 | | H H | N C |
| | ATOM ATOM | 2050 | CA | SER H | 52 | -12.333 | 10.368 | -0.060 | 1.00 40.73 | | H | Č |
| 55 | ATOM | 2052 | ŏ | SER H | 52 | -14.793 | 9.998 | 0.712 | 1.00 35.28 | | H | 0 |
| | MOTA | 2053 | CB | SER H | 52 | -12.218 | 9.216 | -1.504 | 1.00 41.62 | | H | C |
| | MOTA | 2054 | OG | SER H | 52 | -13.410 | 8.701 | -2.095 | 1.00 45.13 1.00 47.25 | | H H | O |
| | ATOM ATOM | 2055 2056 | N CA | SER H SER H | 53 53 | -14.093 -15.357 | 11.396 12.121 | -0.908 -0.908 | 1.00 47.25 | | H | C N |
| 60 | ATOM | 2057 | C | SER H | 53 | -16.543 | 11.198 | -1.204 | 1.00 49.75 | | H | Č |
| | MOTA | 2058 | 0 | SER H | 53 | -17.655 | 11.384 | -0.725 | 1.00 53.93 | | H | 0 |
| | ATOM | 2059 | CB | SER H | 53 | -15.271 | 13.217 | -1.969 | 1.00 52.83 | | H | C |
| | ATOM | 2060 | OG | SER H | 53 | -14.297 -16.279 | 14.184 10.189 | -1.575 -2.056 | 1.00 58.40 1.00 45.24 | | H H | <i>N</i> O |
| 65 | ATOM ATOM | 2061 2062 | N CA | GLY H | 54 54 | -10.279 -17.355 | 9.296 | -2.474 | 1.00 43.24 | | H | C |
| - | ATOM | 2063 | C | GLY H | 54 | -17.537 | 8.118 | -1.512 | 1.00 55.63 | 3 | H | С |
| | ATOM | 2064 | 0 | GLY H | 54 | -18.380 | 7.250 | -1.697 | 1.00 61.25 | | H | O |
| | MOTA | 2065 | N | GLY H | 55 55 | -16.673 | 8.082 | $-0.479 \\ 0.505$ | 1.00 53.22 1.00 54.53 | | H H | N C |
| | ATOM | 2066 | CA | GLY H | 55 | -16.775 | 7.009 | 0.505 | 1.00 34.5. | • | 11 | |

| | MOTA | 2067 | С | GLY H | 55 | -16.009 | 5.760 | 0.062 | 1.00 55.03 | F | H C |
|----|------|------|------------------|-------|----|-----------------|--------|--------|------------|--------|--------------|
| | ATOM | 2068 | 0 | GLY H | 55 | -16.062 | 4.710 | 0.688 | 1.00 63.61 | F | |
| | MOTA | 2069 | N | ASN H | 56 | -15.076 | 5.866 | -0.905 | 1.00 50.20 | F | - |
| | ATOM | 2070 | CA | ASN H | 56 | -14.132 | 4.775 | -1.117 | 1.00 53.18 | | i C |
| 5 | MOTA | 2071 | C | ASN H | 56 | -13.066 | 4.733 | -0.020 | 1.00 51.97 | | H C |
| J | ATOM | 2072 | | ASN H | 56 | | 5.729 | 0.321 | 1.00 52.37 | | |
| | | | O | | | -12.441 | | | | F | |
| | MOTA | 2073 | CB | ASN H | 56 | -13.471 | 4.973 | -2.482 | 1.00 61.77 | | H C |
| | MOTA | 2074 | CG | ASN H | 56 | -14.484 | 4.728 | -3.571 | 1.00 70.16 | ŀ | |
| | MOTA | 2075 | | ASN H | 56 | -14.773 | 5.591 | -4.395 | 1.00 79.19 | | 1 O |
| 10 | MOTA | 2076 | | ASN H | 56 | -15.032 | 3.501 | -3.570 | 1.00 83.81 | ŀ | |
| | MOTA | 2077 | \boldsymbol{N} | THR H | 57 | -12.896 | 3.534 | 0.568 | 1.00 48.61 | F | ı N |
| | MOTA | 2078 | ca | THR H | 57 | -11.950 | 3.401 | 1.670 | 1.00 40.92 | F | H C |
| | ATOM | 2079 | C | THR H | 57 | -10.671 | 2.672 | 1.248 | 1.00 38.31 | F | I C |
| | MOTA | 2080 | 0 | THR H | 57 | -10.627 | 1.959 | 0.254 | 1.00 40.67 | F | O E |
| 15 | MOTA | 2081 | CB | THR H | 57 | -12.638 | 2.631 | 2.801 | 1.00 40.83 | F | |
| | MOTA | 2082 | OG1 | | 57 | -13.012 | 1.335 | 2.329 | 1.00 42.11 | F | |
| | MOTA | 2083 | CG2 | | 57 | -13.899 | 3.379 | 3.251 | 1.00 23.85 | | i Č |
| | MOTA | 2084 | N | TYR H | 58 | -9.590 | 2.906 | 1.978 | 1.00 40.21 | | H N |
| | MOTA | 2085 | CA | TYR H | 58 | -8.307 | 2.302 | 1.653 | 1.00 38.47 | ŀ | |
| 20 | ATOM | 2086 | CA | TYR H | 58 | -7.600 | 2.013 | 2.962 | 1.00 37.26 | | |
| 20 | | | | | | -7.653 | 2.816 | 3.888 | | | |
| | MOTA | 2087 | O | TYR H | 58 | | | | 1.00 39.78 | | OF |
| | ATOM | 2088 | CB | TYR H | 58 | -7.448 | 3.246 | 0.803 | 1.00 37.94 | | H C |
| | MOTA | 2089 | CG | TYR H | 58 | -8.165 | 3.856 | -0.374 | 1.00 45.00 | | H C |
| | MOTA | 2090 | CD1 | | 58 | -9.022 | 4.937 | -0.200 | 1.00 38.69 | | H C |
| 25 | MOTA | 2091 | CD2 | | 58 | -7.996 | 3.350 | -1.661 | 1.00 42.28 | | H C |
| | MOTA | 2092 | CE1 | | 58 | -9.688 | 5.497 | -1.265 | 1.00 48.56 | F | |
| | MOTA | 2093 | CE2 | TYR H | 58 | -8.664 | 3.904 | -2.737 | 1.00 45.82 | F | H C |
| | MOTA | 2094 | CZ | TYR H | 58 | -9.510 | 4.979 | -2.531 | 1.00 50.99 | ŀ | I C |
| | MOTA | 2095 | OH | TYR H | 58 | -10.205 | 5.537 | -3.582 | 1.00 45.05 | F | OF |
| 30 | MOTA | 2096 | N | TYR H | 59 | ~6.923 | 0.871 | 3.023 | 1.00 38.15 | F | H N |
| | ATOM | 2097 | CA | TYR H | 59 | -6.228 | 0.448 | 4.229 | 1.00 36.23 | | H C |
| | MOTA | 2098 | C | TYR H | 59 | -4.923 | -0.272 | 3.956 | 1.00 35.97 | | H C |
| | ATOM | 2099 | Ö | TYR H | 59 | -4.744 | -0.877 | 2.910 | 1.00 41.66 | | i O |
| | MOTA | 2100 | СВ | TYR H | 59 | -7.114 | -0.521 | 4.990 | 1.00 32.92 | | H C |
| 35 | ATOM | 2101 | CG | TYR H | 59 | -8.483 | 0.001 | 5.308 | 1.00 33.05 | | H C |
| 33 | | | | | | | | | | | |
| | MOTA | 2102 | CD1 | | 59 | -8.692 | 0.811 | 6.410 | 1.00 26.16 | | H C |
| | MOTA | 2103 | CD2 | | 59 | -9.578 | -0.351 | 4.531 | 1.00 21.88 | | H C |
| | ATOM | 2104 | CE1 | | 59 | -9.949 | 1.248 | 6.738 | 1.00 28.20 | | H C |
| | MOTA | 2105 | CE2 | | 59 | -10.839 | 0.087 | 4.851 | 1.00 30.66 | | H C |
| 40 | ATOM | 2106 | CZ | TYR H | 59 | -11.018 | 0.883 | 5.961 | 1.00 27.82 | ŀ | H C |
| | MOTA | 2107 | oh | TYR H | 59 | -12.274 | 1.296 | 6.325 | 1.00 47.49 | F | O E |
| | MOTA | 2108 | N | PRO H | 60 | ~3.983 | -0.209 | 4.901 | 1.00 42.07 | F | \mathbf{N} |
| | MOTA | 2109 | CA | PRO H | 60 | -2.717 | -0.912 | 4.691 | 1.00 42.47 | F | i C |
| | MOTA | 2110 | C | PRO H | 60 | -3.021 | -2.380 | 5.039 | 1.00 42.12 | F | H C |
| 45 | MOTA | 2111 | 0 | PRO H | 60 | -3.990 | -2.667 | 5.748 | 1.00 34.35 | F | OF |
| | MOTA | 2112 | CB | PRO H | 60 | -1.787 | -0.282 | 5.728 | 1.00 37.68 | F | T C |
| | ATOM | 2113 | CG | PRO H | 60 | -2.423 | 0.998 | 6.070 | 1.00 38.55 | | i C |
| | MOTA | 2114 | CD | PRO H | 60 | -3.881 | 0.718 | 6.039 | 1.00 41.23 | | i C |
| | ATOM | 2115 | N | ASP H | 61 | -2.213 | -3.314 | 4.556 | 1.00 46.33 | Ī | |
| 50 | MOTA | 2116 | CA | ASP H | 61 | -2.466 | -4.702 | 4.904 | 1.00 53.50 | F | |
| 00 | ATOM | 2117 | C | ASP H | 61 | -2.319 | -4.842 | 6.415 | 1.00 52.80 | ŀ | |
| | | 2118 | | | 61 | -2.773 | -5.818 | | 1.00 52.80 | | 1 0 |
| | MOTA | | O | ASP H | | | | 7.006 | | F | |
| | MOTA | 2119 | CB | ASP H | 61 | -1.467 | -5.625 | 4.219 | 1.00 56.53 | ŀ | |
| | MOTA | 2120 | CG | ASP H | 61 | -1.512 | -5.513 | 2.722 | 1.00 72.07 | F | |
| 55 | MOTA | 2121 | | ASP H | 61 | -2.632 | -5.429 | 2.161 | 1.00 70.71 | F | |
| | MOTA | 2122 | OD2 | ASP H | 61 | -0.421 | -5.524 | 2.110 | 1.00 91.21 | F | 4 O |
| | MOTA | 2123 | N | SER H | 62 | -1.672 | -3.849 | 7.016 | 1.00 52.97 | F | H N |
| | MOTA | 2124 | CA | SER H | 62 | -1.359 | -3.808 | 8.438 | 1.00 48.81 | F | I C |
| | MOTA | 2125 | С | SER H | 62 | -2.619 | -3.866 | 9.309 | 1.00 49.13 | F | |
| 60 | MOTA | 2126 | 0 | SER H | 62 | -2.612 | -4.355 | 10.431 | 1.00 48.28 | F | |
| | MOTA | 2127 | ĊВ | SER H | 62 | -0.589 | -2.516 | 8.718 | 1.00 50.55 | - F | |
| | ATOM | 2128 | ŌĠ | SER H | 62 | -0.528 | -2.299 | 10.127 | 1.00 60.82 | F | |
| | ATOM | 2129 | N | VAL H | 63 | -3.723 | -3.309 | 8.770 | 1.00 45.57 | ŀ | |
| | ATOM | 2130 | CA | VAL H | 63 | -4.947 | -3.243 | 9.562 | 1.00 39.30 | ŀ | |
| 65 | ATOM | 2131 | CA | VAL H | 63 | -6.183 | -3.685 | 8.770 | 1.00 37.75 | F | |
| 55 | | 2132 | | | | | -3.711 | 9.267 | | | |
| | MOTA | | O CP | VAL H | 63 | -7.301 E 120 | | | 1.00 37.52 | I- | |
| | MOTA | 2133 | CB | VAL H | 63 | -5.128 | -1.800 | 10.039 | 1.00 42.39 | F | |
| | MOTA | 2134 | | VAL H | 63 | -3.887 | -1.349 | 10.809 | 1.00 34.90 | F | |
| | MOTA | 2135 | CG2 | VAL H | 63 | -5.337 | -0.882 | 8.849 | 1.00 31.97 | F | G C |

| | ATOM ATOM | 2136 2137 | N CA | LYS H LYS H | 64 64 | -5.959 | ~4.004 | 7.482 | 1.00 40.88 | Н | N |
|----|--------------|---------------------|------------|----------------|----------|--------------------|------------------|-------------------|--------------------------|--------|--------|
| | ATOM | 2138 | CA | LYS H | 64 | -7.068 -7.836 | -4.431 -5.603 | 6.636 7.254 | 1.00 47.29 1.00 47.68 | H H | C |
| _ | ATOM | 2139 | 0 | LYS H | 64 | -7.266 | -6.604 | 7.666 | 1.00 46.11 | H | 0 |
| 5 | MOTA MOTA | $2140 \\ 2141$ | CB CG | LYS H LYS H | 64 64 | -6.501 -7.097 | ~4.839 ~4.021 | 5.275 4.128 | 1.00 49.64 1.00 59.25 | H H | C |
| | ATOM | 2142 | CD | LYS H | 64 | -6.884 | -4.688 | 2.768 | 1.00 71.56 | H | č |
| | ATOM | 2143 | CE | LYS H | 64 | -5.402 | -4.805 | 2.398 | 1.00 81.53 | H | C |
| 10 | ATOM ATOM | $2144 \\ 2145$ | NZ N | LYS H GLY H | 64 65 | -4.916 -9.165 | -3.520 -5.387 | $1.899 \\ 7.295$ | 1.00 49.44 1.00 47.28 | H H | N |
| 10 | MOTA | 2146 | CA | GLY H | 65 | -10.047 | -6.409 | 7.845 | 1.00 47.28 | H | C N |
| | MOTA | 2147 | C | GLY H | 65 | -10.249 | -6.226 | 9.351 | 1.00 42.83 | H | С |
| | ATOM ATOM | 2148 2149 | N O | GLY H ARG H | 65 66 | -11.115 -9.381 | -6.832 -5.381 | 9.971 9.942 | 1.00 50.95 1.00 43.96 | H | 0 |
| 15 | MOTA | 2150 | CA | ARG H | 66 | -9.459 | -5.142 | 11.380 | 1.00 43.96 | H H | C M |
| | ATOM | 2151 | Ç | ARG H | 66 | -9.991 | -3.739 | 11.703 | 1.00 43.62 | H | C |
| | ATOM ATOM | 2152 2153 | O CB | ARG H ARG H | 66 66 | -10.440 | -3.458 -5.306 | 12.806 11.960 | 1.00 49.65 | H | 0 |
| | ATOM | $\frac{2153}{2154}$ | CG | ARG H | 66 | -8.054 -7.998 | -6.360 | 13.065 | 1.00 46.94 1.00 35.48 | H H | C |
| 20 | ATOM | 2155 | CD | ARG H | 66 | -6.616 | -7.012 | 13.160 | 1.00 36.46 | H | C |
| | ATOM ATOM | 2156 2157 | $_{ m CZ}$ | ARG H ARG H | 66 66 | -5.577 -5.142 | -6.084 -5.162 | 12.704 13.584 | 1.00 43.95 | H | N |
| | ATOM | 2158 | | ARG H | 66 | -5.142 -5.650 | -5.116 | 13.384 14.802 | 1.00 50.13 1.00 43.60 | H H | N |
| | MOTA | 2159 | | ARG H | 66 | -4.169 | -4.317 | 13.229 | 1.00 44.39 | H | N |
| 25 | MOTA MOTA | 2160 2161 | N CA | PHE H | 67 67 | -9.864 -10.226 | -2.799 -1.396 | 10.773 10.999 | 1.00 44.77 | H | И |
| | ATOM | 2162 | CA | PHE H | 67 | -11.197 | -0.910 | 9.919 | 1.00 40.21 1.00 41.98 | H H | C |
| | ATOM | 2163 | 0 | PHE H | 67 | -11.115 | ~1.327 | 8.755 | 1.00 40.85 | H | 0 |
| 30 | ATOM ATOM | 2164 2165 | CB CG | PHE H PHE H | 67 67 | -8.972 | ~0.505 | 10.932 | 1.00 35.58 | H | C |
| 30 | ATOM | 2166 | | PHE H | 67 67 | -8.052 -7.966 | -0.631 -1.803 | 12.101 12.826 | 1.00 34.08 1.00 46.65 | H H | C |
| | ATOM | 2167 | CD2 | PHE H | 67 | -7.234 | 0.428 | 12.457 | 1.00 34.35 | H | C |
| | MOTA | 2168 | | PHE H | 67 | -7.074 | -1.916 | 13.890 | 1.00 47.26 | H | C |
| 35 | MOTA MOTA | 2169 2170 | CE2 CZ | PHE H PHE H | 67 67 | -6.344 -6.263 | 0.327 -0.847 | 13.512 14.231 | 1.00 28.12 1.00 36.89 | H H | C |
| | ATOM | 2171 | N | THR H | 68 | -12.103 | -0.015 | 10.294 | 1.00 36.98 | H | й |
| | ATOM | 2172 | CA | THR H | 68 | -12.990 | 0.490 | 9.266 | 1.00 39.60 | H | C |
| | ATOM ATOM | 2173 2174 | C O | THR H | 68 68 | -13.142 -13.517 | $1.991 \\ 2.515$ | $9.400 \\ 10.441$ | 1.00 37.70 1.00 33.56 | H H | 0 |
| 40 | MOTA | 2175 | СВ | THR H | 68 | -14.353 | -0.178 | 9.438 | 1.00 38.69 | H | č |
| | ATOM | 2176 | OG1 | | 68 | -14.194 | -1.595 | 9.356 | 1.00 38.20 | H | 0 |
| | ATOM ATOM | 2177 2178 | N N | THR H | 68 69 | -15.300 -12.783 | 0.271 2.695 | 8.319 8.317 | 1.00 40.05 1.00 35.22 | H H | N C |
| | ATOM | 2179 | CA | ILE H | 69 | -12.986 | 4.133 | 8.310 | 1.00 33.39 | H | Č |
| 45 | ATOM | 2180 | C | ILE H | 69 | -14.365 | 4.494 | 7.763 | 1.00 29.12 | H | C |
| | MOTA MOTA | 2181 2182 | O CB | ILE H ILE H | 69 69 | -14.922 -11.907 | $3.843 \\ 4.772$ | 6.887 7.441 | 1.00 35.88 1.00 27.05 | H H | 0 |
| | ATOM | 2183 | | ILE H | 69 | -12.088 | 6.295 | 7.426 | 1.00 28.35 | H | č |
| F0 | ATOM | 2184 | | ILE H | 69 | -12.050 | 4.263 | 5.996 | 1.00 39.66 | H | C |
| 50 | ATOM ATOM | 2185 2186 | N | ILE H SER H | 69 70 | -10.819 -14.928 | 7.041 5.556 | 7.837 8.356 | 1.00 19.70 1.00 30.01 | H H | N C |
| | MOTA | 2187 | ĈA. | SER H | 70 | -16.200 | 6.073 | 7.882 | 1.00 32.13 | H | Ĉ |
| | ATOM | 2188 | C | SER H | 70 | -16.299 | 7.561 | 8.199 | 1.00 36.01 | H | C |
| 55 | ATOM ATOM | 2189 2190 | O CB | SER H SER H | 70 70 | -15.622 -17.325 | 8.076 5.310 | 9.079 8.588 | 1.00 41.38 1.00 25.57 | H H | C |
| | ATOM | 2191 | OG | SER H | 70 | -17.077 | 5.312 | 9.995 | 1.00 41.99 | H | ŏ |
| | ATOM | 2192 | N | ARG H | 71 | -17.245 | 8.171 | 7.500 | 1.00 35.84 | H | N |
| | MOTA MOTA | $2193 \\ 2194$ | CA C | ARG H ARG H | 71 71 | -17.510 -18.987 | 9.585 9.900 | 7.679 7.764 | 1.00 34.27 1.00 33.22 | H H | C |
| 60 | ATOM | 2195 | Õ | ARG H | 71 | -19.806 | 9.240 | 7.142 | 1.00 35.22 | H | ŏ |
| | ATOM | 2196 | CB | ARG H | 71 | -16.894 | 10.356 | 6.508 | 1.00 31.22 | H | C |
| | ATOM ATOM | 2197 2198 | CG CD | ARG H ARG H | 71 71 | -17.360 -16.570 | 9.860 10.499 | 5.147 4.049 | 1.00 24.64 1.00 24.11 | H H | C C |
| | ATOM | 2199 | NE | ARG H | 71 | -16.406 | 11.925 | 4.319 | 1.00 24.11 | H | N |
| 65 | MOTA | 2200 | CZ | ARG H | 71 | -15.497 | 12.703 | 3.739 | 1.00 13.51 | H | C |
| | MOTA MOTA | 2201 2202 | | ARG H ARG H | 71 71 | -14.654 -15.416 | 12.209 13.972 | $2.838 \\ 4.090$ | 1.00 21.43 1.00 32.61 | H H | N |
| | ATOM | 2203 | N | ASP H | 72 | -19.324 | 10.907 | 8.556 | 1.00 37.54 | H | N |
| | MOTA | 2204 | CA | ASP H | 72 | -20.700 | 11.355 | 8.676 | 1.00 37.74 | н | C |
| | | | | | | | | | | | |

| | - | | | | | | | | | | | |
|----|-----------------|------|---------|-------|------|---------|--------|---------|------------|----|--------|---|
| | ATOM | 2205 | С | ASP H | 72 | -20.669 | 12.790 | 0 1 1 1 | 1 00 26 70 | | | |
| | ATOM | 2206 | | | | | | 8.141 | 1.00 36.70 | | H | С |
| | | | 0 | ASP H | 72 | -20.260 | 13.724 | 8.842 | 1.00 29.75 | | H | 0 |
| | ATOM | 2207 | CB | ASP H | 72 | -21.150 | 11.342 | 10.129 | 1.00 41.57 | | H | С |
| | ATOM | 2208 | CG | ASP H | 72 . | -22.622 | 11.677 | 10.284 | 1.00 48.19 | | H | C |
| 5 | ATOM | 2209 | OD1 | ASP H | 72 | -23.145 | 12.522 | 9.518 | 1.00 49.97 | | H | ŏ |
| | ATOM | 2210 | | ASP H | 72 | -23.257 | 11.103 | 11.194 | | | | |
| | ATOM | | | | | | | | 1.00 56.29 | | H | 0 |
| | | 2211 | N | ASN H | 73 | -21.077 | 12.950 | 6.884 | 1.00 36.00 | | H | N |
| | ATOM | 2212 | ca | ASN H | 73 | -21.075 | 14.252 | 6.237 | 1.00 34.23 | | H | С |
| | ATOM | 2213 | C | ASN H | 73 | -22.025 | 15.261 | 6.837 | 1.00 38.06 | | H | Č |
| 10 | ATOM | 2214 | 0 | ASN H | 73 | -21.655 | 16.419 | 7.034 | 1.00 42.98 | | H | |
| | ATOM | 2215 | СВ | ASN H | 73 | -21.341 | | | | | | 0 |
| | | | | | | | 14.098 | 4.748 | 1.00 35.94 | | H | C |
| | ATOM | 2216 | | ASN H | 73 | -20.148 | 13.534 | 4.017 | 1.00 28.67 | | H | С |
| | ATOM | 2217 | OD1 | ASN H | 73 | -19.034 | 13.567 | 4.523 | 1.00 38.30 | | H | 0 |
| | ATOM | 2218 | ND2 | ASN H | 73 | -20.369 | 13.027 | 2.817 | 1.00 40.69 | | H | N |
| 15 | ATOM | 2219 | N | ALA H | 74 | -23.246 | 14.837 | 7.135 | 1.00 40.21 | | | |
| | ATOM | 2220 | | ALA H | 74 | | | | | | H | N |
| | | | | | | -24.205 | 15.747 | 7.736 | 1.00 39.70 | | H | C |
| | ATOM | 2221 | | ALA H | 74 | -23.633 | 16.275 | 9.046 | 1.00 43.05 | | H | C |
| | ATOM | 2222 | 0 | ALA H | 74 | -23.592 | 17.484 | 9.275 | 1.00 44.60 | | H | 0 |
| | ATOM | 2223 | CB | ALA H | 74 | -25.509 | 15.038 | 7.988 | 1.00 42.51 | | H | Č |
| 20 | ATOM | 2224 | | ARG H | 75 | -23.173 | 15.364 | 9.900 | | | | |
| | ATOM | 2225 | | | | | | | 1.00 43.49 | | H | N |
| | | _ | | ARG H | 75 | -22.618 | 15.759 | 11.190 | 1.00 40.90 | | H | C |
| | ATOM | 2226 | | ARG H | 75 | -21.177 | 16.231 | 11.119 | 1.00 37.75 | | H | С |
| | ATOM | 2227 | 0 | ARG H | 75 | -20.691 | 16.835 | 12.072 | 1.00 33.26 | | H | Ō |
| | ATOM | 2228 | CB | ARG H | 75 | -22.701 | 14.607 | 12.201 | 1.00 45.03 | | H | |
| 25 | ATOM | 2229 | | ARG H | 75 | -24.098 | | | | | | C |
| 20 | | | | | | | 14.287 | 12.709 | 1.00 61.37 | | H | С |
| | ATOM | 2230 | | ARG H | 75 | -24.062 | 13.295 | 13.873 | 1.00 60.10 | | H | C |
| | ATOM | 2231 | | ARG H | 75 | -23.498 | 13.905 | 15.074 | 1.00 78.94 | 1 | H | N |
| | ATOM | 2232 | CZ | ARG H | 75 | -23.312 | 13.272 | 16.232 | 1.00 84.66 | | H | C |
| | ATOM | 2233 | NH1 | ARG H | 75 | -22.787 | 13.929 | 17.268 | 1.00 58.25 | | | |
| 30 | ATOM | 2234 | | ARG H | 75 | -23.647 | | | | | H | N |
| 00 | | | | | | | 11.988 | 16.357 | 1.00 80.63 | | H | N |
| | ATOM | 2235 | | ASN H | 76 | -20.504 | 15.964 | 9.999 | 1.00 35.22 |] | H | N |
| | ATOM | 2236 | CA | ASN H | 76 | -19.094 | 16.334 | 9.829 | 1.00 33.97 | 1 | H | C |
| | ATOM | 2237 | C | ASN H | 76 | -18.212 | 15.584 | 10.823 | 1.00 36.07 | | H | Č |
| | ATOM | 2238 | | ASN H | 76 | -17.391 | 16.184 | 11.516 | | | | |
| 35 | ATOM | 2239 | | | | | | | 1.00 35.74 | | H | 0 |
| 55 | | | | ASN H | 76 | -18.884 | 17.834 | 10.030 | 1.00 32.35 |] | H | C |
| | MOTA | 2240 | | ASN H | 76 | -19.332 | 18.642 | 8.847 | 1.00 38.66 |] | H | C |
| | ATOM | 2241 | OD1 | ASN H | 76 | -18.695 | 19.630 | 8.474 | 1.00 45.80 | 1 | H | 0 |
| | ATOM | 2242 | ND2 | ASN H | 76 | -20.423 | 18.221 | 8.231 | 1.00 48.96 | | H | N |
| | ATOM | 2243 | | ILE H | 77 | -18.390 | | | | | | |
| 40 | | | | | | | 14.272 | 10.898 | 1.00 36.71 | | H | N |
| 40 | ATOM | 2244 | | ILE H | 77 | -17.600 | 13.476 | 11.804 | 1.00 32.46 | J | H | C |
| | ATOM | 2245 | C | ILE H | 77 | -16.944 | 12.340 | 11.050 | 1.00 35.64 | J | F | C |
| | MOTA | 2246 | 0 | ILE H | 77 | -17.548 | 11.725 | 10.174 | 1.00 35.33 | | H | ō |
| | MOTA | 2247 | | ILE H | 77 | -18.464 | 12,901 | 12.946 | 1.00 40.83 | | | |
| | ATOM | 2248 | | ILE H | 77 | | | | | | H | C |
| 45 | | | | | | -19.212 | 14.038 | 13.651 | 1.00 44.32 | 1 | F | C |
| 45 | ATOM | 2249 | | ILE H | 77 | -17.578 | 12.170 | 13.962 | 1.00 40.40 | I | Ŧ | С |
| | \mathbf{ATOM} | 2250 | CD1 | ILE H | 77 | -20.069 | 13.586 | 14.813 | 1.00 46.94 | F | H | C |
| | MOTA | 2251 | N | LEU H | 78 | -15.692 | 12.079 | 11.406 | 1.00 40.62 | | - H | N |
| | ATOM | 2252 | | LEU H | 78 | -14.882 | 11.020 | 10.806 | 1.00 37.20 | | | |
| | ATOM | 2253 | | LEU H | | | | 11 054 | | | F | C |
| ~0 | | | | | 78 | -14.783 | 9.910 | 11.854 | 1.00 36.25 | | F | C |
| 50 | MOTA | 2254 | | LEU H | 78 | -14.611 | 10.187 | 13.039 | 1.00 41.81 | F | Ŧ | 0 |
| | ATOM | 2255 | CB : | LEU H | 78 | -13.486 | 11.575 | 10.478 | 1.00 30.31 | I | Ŧ | C |
| | MOTA | 2256 | CG : | LEU H | 78 | -12.471 | 10.688 | 9.765 | 1.00 14.90 | | Ī | č |
| | MOTA | 2257 | | LEU H | 78 | -12.957 | 10.314 | 8.404 | | | | ä |
| | | | | | | | | | 1.00 28.76 | F | | C |
| ~- | MOTA | 2258 | CDZ . | LEU H | 78 | -11.163 | 11.414 | 9.673 | 1.00 31.63 | F | Ŧ | С |
| 55 | ATOM | 2259 | N ' | TYR H | 79 | -14.885 | 8.658 | 11.426 | 1.00 35.10 | F | I | N |
| | ATOM | 2260 | CA ' | TYR H | 79 | -14.814 | 7.539 | 12.364 | 1.00 29.30 | I | | C |
| | ATOM | 2261 | | TYR H | 79 | -13.764 | 6.504 | 12.031 | 1.00 29.91 | Ī | | |
| | ATOM | 2262 | | TYR H | 79 | -13.455 | | | | | | C |
| | | | | | | | 6.258 | 10.864 | 1.00 32.26 | F | | 0 |
| 00 | MOTA | 2263 | | TYR H | 79 | -16.155 | 6.803 | 12.428 | 1.00 28.95 | F | I | C |
| 60 | ATOM | 2264 | | TYR H | 79 | -17.303 | 7.636 | 12.910 | 1.00 37.13 | F | I | C |
| | MOTA | 2265 | | TYR H | 79 | -17.389 | 8.038 | 14.236 | 1.00 19.81 | F | | č |
| | ATOM | 2266 | | TYR H | 79 | -18.290 | 8.047 | 12.030 | 1.00 36.50 | | | 2 |
| | MOTA | 2267 | | | | 10 400 | | | | F | | C |
| | | | | TYR H | 79 | -18.426 | 8.830 | 14.668 | 1.00 44.55 | F | | С |
| 05 | ATOM | 2268 | | TYR H | 79 | -19.333 | 8.841 | 12.453 | 1.00 35.59 | F | I | C |
| 65 | MOTA | 2269 | CZ (| TYR H | 79 | -19.401 | 9.230 | 13.769 | 1.00 40.18 | F | | C |
| | ATOM | 2270 | | TYR H | 79 | -20.456 | 10.014 | 14.181 | 1.00 44.04 | F | | ŏ |
| | MOTA | 2271 | | LEU H | 80 | -13.221 | 5.897 | 13.076 | | | | |
| | MOTA | | | | | | | | 1.00 32.78 | F | | Ñ |
| | | 2272 | | LEU H | 80 | -12.272 | 4.816 | 12.911 | 1.00 33.37 | I. | i | C |
| | MOTA | 2273 | C I | LEU H | 80 | -12.681 | 3.719 | 13.889 | 1.00 39.11 | F | I | C |
| | | | | | | | | | | | | |

| | MOTA MOTA MOTA | 2274 2275 2276 | O LEU H CB LEU H CG LEU H | 80 | -12.510 -10.833 -9.905 | 3.861 5.248 4.066 | 15.100 13.202 12.850 | 1.00 42.27 1.00 27.32 1.00 29.89 | Н Н Н | 0 C |
|----|--|--|---|------------------------------|--|--|--|--|-----------------------|---|
| 5 | ATOM ATOM ATOM | 2277 2278 2279 | CD1 LEU F CD2 LEU F N GLN F | H 80 H 81 | -10.141 -8.445 -13.261 | 3.684 4.396 2.641 | 11.396 13.096 13.368 | 1.00 29.23 1.00 21.87 1.00 37.58 | H H H | С С С |
| 10 | ATOM ATOM ATOM ATOM ATOM ATOM | 2280 2281 2282 2283 2284 2285 | CA GLN F C GLN F C GLN F CB GLN F CG GLN F CD GLN F | H 81 H 81 H 81 H 81 | -13.588 -12.477 -11.955 -14.898 -15.181 -16.017 | 1.586 0.589 0.295 0.949 -0.381 -0.128 | 14.268 14.176 13.108 13.804 14.504 15.737 | 1.00 35.42 1.00 35.75 1.00 38.97 1.00 32.22 1.00 46.99 1.00 63.73 | н н н н н | |
| 15 | ATOM ATOM ATOM ATOM ATOM | 2286 2287 2288 2289 2290 | OE1 GLN H NE2 GLN H N MET H CA MET H C MET H | 81 82 82 | -16.772 -15.848 -12.046 -10.916 -11.369 | 0.824 -1.048 0.146 -0.759 -2.034 | 15.842 16.707 15.350 15.462 16.171 | 1.00 73.22 1.00 54.60 1.00 38.89 1.00 38.00 1.00 41.10 | H H H H | C N O |
| 20 | ATOM ATOM ATOM ATOM ATOM | 2291 2292 2293 2294 2295 | O MET H CB MET H CG MET H SD MET H CE MET H | 82 82 82 | -12.060 -9.786 -9.219 -7.917 -8.890 | -1.982 -0.079 1.170 1.992 2.540 | 17.192 16.236 15.554 16.522 17.888 | 1.00 42.49 1.00 40.92 1.00 40.95 1.00 43.01 1.00 36.86 | н н н н | 000000000000000000000000000000000000000 |
| 25 | ATOM ATOM ATOM ATOM ATOM | 2296 2297 2298 2299 2300 | N SER H CA SER H C SER H O SER H CB SER H | 82A 82A 82A 82A | -10.994 -11.395 -10.238 -9.323 | -3.182 -4.446 -5.431 -5.335 | 15.621 16.214 16.242 15.431 | 1.00 39.35 1.00 42.12 1.00 43.14 1.00 41.79 | н н н н | N C O |
| 30 | ATOM ATOM ATOM ATOM | 2301 2302 2303 2304 | OG SER H N SER H CA SER H C SER H | 82A 82B 82B 82B | -12.561 -12.101 -10.293 -9.247 -7.940 | -5.052 -5.716 -6.381 -7.383 -6.652 | 15.428 14.258 17.173 17.304 17.535 | 1.00 42.50 1.00 50.18 1.00 40.74 1.00 45.65 1.00 44.33 | Н Н Н Н | C O N C C |
| 35 | ATOM ATOM ATOM ATOM ATOM | 2305 2306 2307 2308 2309 | O SER H CB SER H OG SER H N LEU H CA LEU H | 82B 82B 82C 82C | -6.946 -9.129 -10.320 -7.934 -6.730 | -6.935 -8.213 -8.914 -5.717 -4.932 | 16.866 16.018 15.721 18.480 18.739 | 1.00 51.78 1.00 44.47 1.00 53.60 1.00 40.37 1.00 44.23 | Н Н Н Н | 0 C O |
| 40 | ATOM ATOM ATOM ATOM ATOM | 2310 2311 2312 2313 2314 | C LEU H O LEU H CB LEU H CG LEU H CD1 LEU H | 82C 82C 82C | -5.498 -5.581 -7.032 -7.982 -8.308 | -5.720 -6.625 -3.824 -2.753 -1.699 | 19.171 19.992 19.756 19.194 20.243 | 1.00 42.91 1.00 48.40 1.00 47.83 1.00 48.91 1.00 42.50 | H H H H | מסטטט |
| 45 | ATOM ATOM ATOM ATOM ATOM | 2315 2316 2317 2318 2319 | CD2 LEU H N ARG H CA ARG H C ARG H O ARG H | 82C 83 83 83 | -7.340 -4.354 -3.055 -2.213 -2.434 | -2.116 -5.361 -5.936 -4.938 -3.735 | 17.969 18.590 18.895 19.694 19.663 | 1.00 41.96 1.00 40.80 1.00 36.37 1.00 35.99 1.00 47.57 | H H H H | C N C |
| 50 | ATOM ATOM ATOM ATOM | 2320 2321 2322 2323 | CB ARG H CG ARG H CD ARG H NE ARG H | 83 83 83 83 | -2.359 -3.236 -2.544 -3.470 | -6.300 -7.145 -7.435 -8.063 | 17.577 16.646 15.304 14.349 | 1.00 47.57 1.00 36.69 1.00 40.16 1.00 34.89 1.00 58.83 | н н н н | О С С |
| 55 | ATOM ATOM ATOM ATOM ATOM | 2324 2325 2326 2327 2328 | CZ ARG H NH1 ARG H NH2 ARG H N SER H CA SER H | 83 83 | -3.033 -1.820 -3.825 -1.201 -0.376 | -8.224 -7.821 -8.810 -5.519 -4.674 | 13.083 12.741 12.177 20.361 | 1.00 64.19 1.00 74.93 1.00 64.50 1.00 41.54 | н н н | C N N |
| | ATOM ATOM ATOM ATOM | 2329 2330 2331 2332 | C SER H O SER H CB SER H OG SER H | | 0.260 0.646 0.759 0.202 | -4.674 -3.585 -2.511 -5.531 -6.382 | 21.201 20.332 20.774 21.817 22.817 | 1.00 46.15 1.00 43.60 1.00 47.14 1.00 41.31 1.00 61.14 | н н н н | 0000 |
| 60 | ATOM ATOM ATOM ATOM | 2333 2334 2335 2336 | N GLU H CA GLU H C GLU H O GLU H | 85 85 85 85 | 0.378 1.098 0.219 0.678 | -3.916 -3.027 -1.927 -1.027 | 19.031 18.121 17.521 16.823 | 1.00 45.78 1.00 44.02 1.00 41.37 1.00 47.91 | н н н н | 0 0 0 |
| 65 | MOTA MOTA MOTA MOTA MOTA | 2337 2338 2339 2340 2341 | CB GLU H CG GLU H CD GLU H OE1 GLU H OE2 GLU H | 85 85 85 85 85 | 1.709 1.944 0.951 0.500 0.597 | -3.873 -5.318 -6.200 -7.173 -5.873 | 17.006 17.438 16.728 17.318 15.599 | 1.00 47.56 1.00 66.27 1.00 83.88 1.00 92.64 1.00 78.20 | H H H H | 00000 |
| | ATOM | 2342 | N ASP H | 86 | -1.099 | -2.034 | 17.767 | 1.00 34.93 | H | N |

| ATOM 2346 CB ASP H 86 | 51 H C 52 H O 58 H O 58 H C 53 H C 53 H C 53 H C 53 H C 53 H C |
|--|--|
| ATOM 2350 N THR H 87 -1.010 0.021 19.375 1.00 28. ATOM 2351 CA THR H 87 -0.869 0.995 20.448 1.00 28. ATOM 2352 C THR H 87 -0.116 2.236 19.965 1.00 25. ATOM 2353 O THR H 87 1.070 2.202 19.660 1.00 29. ATOM 2354 CB THR H 87 -0.080 0.324 21.576 1.00 32. ATOM 2355 OG1 THR H 87 -0.724 -0.899 21.940 1.00 45. | .8 H N .8 H C .3 H C .3 H O .53 H C .72 H O .87 H C .87 H C |
| ATOM 2353 O THR H 87 1.070 2.202 19.660 1.00 29. ATOM 2354 CB THR H 87 -0.080 0.324 21.576 1.00 32. ATOM 2355 OG1 THR H 87 -0.724 -0.899 21.940 1.00 45. | 03 H O 53 H C 72 H O 87 H C 59 H N |
| | 59 H N |
| ATOM 2356 CG2 THR H 87 -0.022 1.242 22.800 1.00 28. 15 ATOM 2357 N ALA H 88 -0.856 3.356 19.858 1.00 30. | |
| ATOM 2358 CA ALA H 88 -0.225 4.581 19.382 1.00 28. ATOM 2359 C ALA H 88 -1.188 5.769 19.418 1.00 27. ATOM 2360 O ALA H 88 -2.368 5.636 19.717 1.00 30. | 71 H C)7 H O |
| ATOM 2361 CB ALA H 88 0.252 4.343 17.949 1.00 23. 20 ATOM 2362 N MET H 89 -0.652 6.953 19.137 1.00 28. ATOM 2363 CA MET H 89 -1.458 8.155 19.096 1.00 25. | 18 H N |
| ATOM 2363 CA MET H 89 -1.458 8.155 19.096 1.00 25. ATOM 2364 C MET H 89 -2.140 8.117 17.736 1.00 23. ATOM 2365 O MET H 89 -1.489 7.900 16.713 1.00 26. | 34 H C |
| ATOM 2366 CB MET H 89 -0.571 9.383 19.192 1.00 19. | 08 H C |
| ATOM 2368 SD MET H 89 -2.161 11.144 20.648 1.00 35. | 92 H S |
| ATOM 2370 N TYR H 90 -3.453 8.295 17.721 1.00 24. | 81 H N |
| ATOM 2371 CA TYR H 90 -4.190 8.274 16.464 1.00 28. 30 ATOM 2372 C TYR H 90 -4.611 9.683 16.032 1.00 35. | 61 H C |
| ATOM 2373 O TYR H 90 -5.294 10.401 16.776 1.00 38. | |
| ATOM 2374 CB TYR H 90 -5.408 7.349 16.583 1.00 26. ATOM 2375 CG TYR H 90 -5.038 5.894 16.487 1.00 21. | |
| ATOM 2376 CD1 TYR H 90 -4.360 5.256 17.523 1.00 21. | 33 H C |
| 35 ATOM 2377 CD2 TYR H 90 -5.308 5.170 15.337 1.00 23. | |
| ATOM 2378 CE1 TYR H 90 -3.957 3.940 17.416 1.00 13. ATOM 2379 CE2 TYR H 90 -4.910 3.853 15.215 1.00 32. | |
| ATOM 2379 CE2 TYR H 90 -4.910 3.853 15.215 1.00 32. ATOM 2380 CZ TYR H 90 -4.235 3.244 16.256 1.00 32. | |
| ATOM 2381 OH TYR H 90 -3.826 1.944 16.120 1.00 31. | 42 H O |
| 40 ATOM 2382 N TYR H 91 -4.199 10.063 14.821 1.00 29 | |
| ATOM 2383 CA TYR H 91 -4.482 11.386 14.277 1.00 27 | |
| ATOM 2384 C TYR H 91 -5.437 11.423 13.105 1.00 30 ATOM 2385 O TYR H 91 -5.311 10.607 12.193 1.00 30 | |
| ATOM 2386 CB TYR H 91 -3.190 12.026 13.781 1.00 25 | |
| 45 ATOM 2387 CG TYR H 91 -2.193 12.378 14.848 1.00 36 | |
| ATOM 2388 CD1 TYR H 91 -2.378 13.493 15.653 1.00 30 ATOM 2389 CD2 TYR H 91 -1.057 11.601 15.049 1.00 24 | |
| ATOM 2389 CD2 TYR H 91 -1.057 11.601 15.049 1.00 24 ATOM 2390 CE1 TYR H 91 -1.471 13.821 16.616 1.00 21 | |
| ATOM 2391 CE2 TYR H 91 -0.149 11.929 16.011 1.00 20 | |
| 50 ATOM 2392 CZ TYR H 91 -0.365 13.039 16.790 1.00 19 | |
| ATOM 2393 OH TYR H 91 0.536 13.375 17.763 1.00 38 ATOM 2394 N CYS H 92 -6.396 12.352 13.120 1.00 34 | |
| ATOM 2394 N CYS H 92 -6.396 12.352 13.120 1.00 34 ATOM 2395 CA CYS H 92 -7.249 12.514 11.941 1.00 39 | |
| ATOM 2396 C CYS H 92 -6.598 13.624 11.120 1.00 31 | 38 H C |
| 55 ATOM 2397 O CYS H 92 -6.025 14.575 11.661 1.00 25 | 53 H O |
| ATOM 2398 CB CYS H 92 -8.737 12.860 12.245 1.00 35 ATOM 2399 SG CYS H 92 -9.256 14.091 13.507 1.00 69 | |
| ATOM 2399 SG CYS H 92 -9.256 14.091 13.507 1.00 69 ATOM 2400 N ALA H 93 -6.644 13.474 9.810 1.00 22 | |
| ATOM 2401 CA ALA H 93 -6.063 14.464 8.942 1.00 23 | 14 H C |
| 60 ATOM 2402 C ALA H 93 -6.899 14.620 7.692 1.00 31 | 52 H C |
| ATOM 2403 O ALA H 93 -7.472 13.654 7.178 1.00 37 | |
| 111,011 11 10 11 11 11 11 11 11 11 11 11 11 | |
| ATOM 2406 CA ARG H 94 -7.718 16.112 5.993 1.00 27 | 88 H C |
| 65 ATOM 2407 C ARG H 94 -6.723 15.771 4.885 1.00 30 | |
| ATOM 2408 O ARG H 94 -5.586 16.244 4.902 1.00 35 | 06 H O |
| ATOM 2409 CB ARG H 94 -8.105 17.583 5.924 1.00 26 ATOM 2410 CG ARG H 94 -9.146 17.905 4.880 1.00 32 | 56 H C 06 H C |
| ATOM 2410 CG ARG H 94 -9.146 17.905 4.880 1.00 32 ATOM 2411 CD ARG H 94 -9.449 19.387 4.883 1.00 29 | |

| | MOTA | 2412 | NE | ARG H | 94 | -8.508 | 20.149 | 4.068 | 1.00 43.56 | H | N |
|----|------|------|--------------|-------|------|--------|--------|---------|------------|---|----------|
| | ATOM | 2413 | CZ | ARG H | | -8.502 | 21.476 | 3.986 | 1.00 30.83 | H | Ċ |
| | MOTA | 2414 | | ARG H | | -9.380 | | | 1.00 32.80 | | |
| | | | | | | | 22.189 | 4.671 | | H | N |
| _ | ATOM | 2415 | | ARG H | | -7.626 | 22.089 | 3.208 | 1.00 26.74 | H | N |
| 5 | MOTA | 2416 | N | LEU H | | -7.134 | 14.922 | 3.949 | 1.00 28.97 | H | N |
| | MOTA | 2417 | CA | LEU H | 95 | -6.369 | 14.534 | 2.771 | 1.00 29.42 | H | C |
| | MOTA | 2418 | C | LEU H | | -6.686 | 15.429 | 1.571 | 1.00 34.07 | H | č |
| | ATOM | 2419 | ŏ | LEU H | | -7.687 | 15.275 | 0.885 | 1.00 43.12 | | |
| | | | | | | | | | | H | 0 |
| | MOTA | 2420 | CB | LEU H | | -6.703 | 13.077 | 2.438 | 1.00 31.81 | H | C |
| 10 | MOTA | 2421 | CG | LEU H | | -5.882 | 12.539 | 1.263 | 1.00 17.92 | H | C |
| | MOTA | 2422 | CD1 | LEU H | 95 | -4.381 | 12.512 | 1.564 | 1.00 33.14 | H | C |
| | MOTA | 2423 | CD2 | LEU H | | -6.265 | 11.111 | 0.872 | 1.00 43.38 | H | . Ç |
| | ATOM | 2424 | | ASP H | | -5.805 | | | | | |
| | | | N | | | | 16.423 | 1.356 | 1.00 33.38 | H | N |
| | MOTA | 2425 | CA | ASP H | | -5.991 | 17.315 | 0.218 | 1.00 26.87 | H | C |
| 15 | MOTA | 2426 | C | ASP H | 96 | -5.736 | 16.588 | -1.105 | 1.00 28.04 | H | С |
| | MOTA | 2427 | 0 | ASP H | 96 | -5.942 | 17.112 | -2.191 | 1.00 31.10 | H | 0 |
| | ATOM | 2428 | CB | ASP H | | -5.021 | 18.489 | 0.367 | 1.00 20.28 | H | č |
| | MOTA | 2429 | CG | ASP H | | -5.550 | 19.449 | 1.425 | | | ~ |
| | | | | | | | | | 1.00 35.23 | H | C |
| | MOTA | 2430 | | ASP H | | -6.142 | 18.967 | 2.392 | 1.00 43.82 | H | 0 |
| 20 | MOTA | 2431 | OD2 | ASP H | 96 | -5.368 | 20.655 | 1.276 | 1.00 34.55 | H | 0 |
| | MOTA | 2432 | N | GLY H | 97 | -5.233 | 15.345 | -0.982 | 1.00 35.21 | H | N |
| | MOTA | 2433 | CA | GLY H | 97 | -4.929 | 14.566 | -2.178 | 1.00 34.98 | H | Ċ |
| | MOTA | 2434 | C | GLY H | | -3.509 | 13.995 | -2.126 | 1.00 36.60 | | ~ |
| | | | | - | | | | | | H | C |
| | ATOM | 2435 | 0 | GLY H | | -2.829 | 14.030 | -1.109 | 1.00 55.18 | H | 0 |
| 25 | MOTA | 2436 | \mathbf{N} | TYR H | 98 | -3.080 | 13.414 | -3.264 | 1.00 31.33 | H | N |
| | MOTA | 2437 | CA | TYR H | 98 | -1.726 | 12.873 | -3.319 | 1.00 36.60 | H | C |
| | MOTA | 2438 | C | TYR H | | -0.732 | 13.899 | -3.869 | 1.00 38.11 | H | Č |
| | ATOM | 2439 | õ | TYR H | | 0.479 | 13.718 | -3.839 | | | |
| | | | | | | | | | 1.00 38.31 | H | 0 |
| | ATOM | 2440 | CB | TYR H | | -1.735 | 11.616 | -4.192 | 1.00 33.71 | H | C |
| 30 | MOTA | 2441 | CG | TYR H | 98 | -2.226 | 11.936 | ~5.559 | 1.00 38.48 | H | ,C |
| | ATOM | 2442 | CD1 | TYR H | 98 | -1.549 | 12.869 | -6.342 | 1.00 60.19 | H | C |
| | MOTA | 2443 | | TYR H | | -3.278 | 11.206 | -6.116 | 1.00 58.17 | H | č |
| | | | | | | | | | | | <u>_</u> |
| | ATOM | 2444 | CE1 | | | -1.902 | 13.051 | -7.672 | 1.00 61.07 | H | C |
| | MOTA | 2445 | CE2 | | | -3.636 | 11.395 | -7.442 | 1.00 66.49 | H | C |
| 35 | MOTA | 2446 | CZ | TYR H | 98 | -2.954 | 12.313 | -8.218 | 1.00 62,63 | H | C |
| | MOTA | 2447 | OH | TYR H | 98 | -3.289 | 12.487 | -9.547 | 1.00 51.32 | H | ō |
| | ATOM | 2448 | N | TYR H | | -1.290 | 14.993 | -4.421 | | | |
| | | | | | | | | | 1.00 34.57 | H | N |
| | MOTA | 2449 | CA | TYR H | | -0.439 | 16.056 | -4.942 | 1.00 28.11 | H | C |
| | ATOM | 2450 | C | TYR H | 99 | 0.077 | 16.958 | -3.819 | 1.00 30.06 | H | C |
| 40 | MOTA | 2451 | 0 | TYR H | 99 | 1.129 | 17.576 | -3.918 | 1.00 45.17 | H | 0 |
| | MOTA | 2452 | СВ | TYR H | | -1.259 | 16.882 | -5.933 | 1.00 35.30 | H | Č |
| | ATOM | 2453 | CG | TYR H | | | | | | | |
| | | | | | | -1.157 | 16.291 | -7.294 | 1.00 45.25 | H | C |
| | MOTA | 2454 | CD1 | | | -2.191 | 16.474 | -8.208 | 1.00 50.19 | H | C |
| | ATOM | 2455 | CD2 | TYR H | 99 | -0.026 | 15.565 | ~7.666 | 1.00 67.32 | H | C |
| 45 | MOTA | 2456 | CE1 | TYR H | 99 | -2.090 | 15.946 | -9.487 | 1.00 61.69 | H | C |
| | MOTA | 2457 | CE2 | | | 0.070 | 15.028 | -8.941 | 1.00 66.78 | H | č |
| | ATOM | 2458 | CZ | TYR H | | -0.958 | 15.211 | | | | |
| | | | | | | | | -9.847 | 1.00 61.53 | H | C |
| | MOTA | 2459 | OH | TYR H | | -0.889 | | -11.107 | 1.00 64.87 | H | 0 |
| | MOTA | 2460 | N | PHE H | 100 | -0.868 | 16.958 | -2.882 | 1.00 28.36 | H | N |
| 50 | MOTA | 2461 | CA | PHE H | 100 | -0.843 | 17.912 | -1.771 | 1.00 33.08 | H | C |
| | ATOM | 2462 | C | PHE H | | -0.564 | 17.528 | -0.313 | 1.00 32.51 | H | Č |
| | ATOM | 2463 | ŏ | PHE H | | -0.409 | 18.414 | 0.510 | | | |
| | | | | | | | | | 1.00 28.93 | H | 0 |
| | MOTA | 2464 | СВ | PHE H | | -2.152 | 18.702 | -1.836 | 1.00 35.07 | H | C |
| | MOTA | 2465 | CG | PHE H | 100 | -2.589 | 19.002 | ~3.244 | 1.00 40.19 | H | C |
| 55 | MOTA | 2466 | CD1 | PHE H | 100 | -1.920 | 19.958 | -4.007 | 1.00 42.98 | H | C |
| | MOTA | 2467 | | PHE H | | -3.604 | 18.264 | -3.841 | 1.00 32.65 | H | Č |
| | ATOM | 2468 | | | | | | | | | |
| | | | | PHE H | | -2.256 | 20.160 | -5.326 | 1.00 38.55 | H | C |
| | MOTA | 2469 | CE2 | PHE H | | -3.942 | 18.464 | -5.164 | 1.00 22.61 | H | C |
| | MOTA | 2470 | $^{\rm cz}$ | PHE H | 100 | -3.272 | 19.407 | ~5.906 | 1.00 34.08 | H | C |
| 60 | ATOM | 2471 | N | GLY H | 100A | -0.513 | 16.243 | 0.023 | 1.00 32.84 | H | N |
| - | MOTA | 2472 | CA | | 100A | -0.246 | 15.859 | 1.403 | 1.00 24.07 | H | Ĉ |
| | | | | | | | | | | | |
| | ATOM | 2473 | Č | | 100A | -1.375 | 15.977 | 2.433 | 1.00 31.86 | H | C |
| | MOTA | 2474 | 0 | | 100A | -2.508 | 16.393 | 2.147 | 1.00 31.43 | H | 0 |
| | MOTA | 2475 | N | PHE H | 100B | -1.062 | 15.565 | 3.656 | 1.00 31.62 | H | N |
| 65 | MOTA | 2476 | CA | | 100B | -2.009 | 15.648 | 4.756 | 1.00 30.23 | H | Ĉ |
| | ATOM | 2477 | C | | 100B | -1.848 | 17.067 | 5.278 | 1.00 28.52 | H | č |
| | | | | | | | | | | | |
| | MOTA | 2478 | 0 | | 100B | -0.932 | 17.358 | 6.045 | 1.00 32.67 | H | 0 |
| | MOTA | 2479 | СВ | | 100B | -1.681 | 14.617 | 5.845 | 1.00 35.30 | H | C |
| | MOTA | 2480 | CG | PHE H | 100B | -1.841 | 13.186 | 5.394 | 1.00 37.11 | H | С |
| | | | | | | | | | | | |

| | ATOM ATOM | 2481 2482 | CD1 PH | | 100B 100B | -0.723 -3.104 | 12.391 12.641 | 5.124 5.211 | 1.00 28.90 1.00 27.19 | | H H | C |
|----|--------------|--------------|----------------|------------|--------------|------------------|-------------------|------------------|--------------------------|---|--------|--------|
| | ATOM | 2483 | | | 100B | -0.864 | 11.089 | 4.682 | 1.00 27.19 | | H | C |
| | ATOM | 2484 | | | 100B | -3.252 | 11.329 | 4.766 | 1.00 27.20 | | H | Č |
| 5 | ATOM | 2485 | | | 100B | -2.136 | 10.556 | 4.502 | 1.00 31.15 | | H | C |
| | MOTA | 2486 | | AH | | -2.758 | 17.933 | 4.833 | 1.00 27.56 | | H | N |
| | ATOM ATOM | 2487 2488 | | AH | | -2.760 -3.142 | 19.355 19.783 | 5.154 6.570 | 1.00 25.66 1.00 25.19 | | H | C |
| | ATOM | 2489 | | AH | | -2.666 | 20.790 | 7.069 | 1.00 25.19 | | H H | C |
| 10 | ATOM | 2490 | | AH | | -3.625 | 20.072 | 4.150 | 1.00 29.91 | | H | Č |
| | MOTA | 2491 | | R H | | -4.008 | 19.038 | 7.226 | 1.00 27.89 | | H | N |
| | ATOM | 2492 | | RH | | -4.398 | 19.414 | 8.574 | 1.00 25.32 | | H | C |
| | MOTA MOTA | 2493 2494 | | RH | | -4.423 -4.814 | 18.174 17.104 | 9.432 8.968 | 1.00 24.39 | | H | C |
| 15 | ATOM | 2495 | | RH | | -5.769 | 20.098 | 8.557 | 1.00 30.42 1.00 23.33 | | H H | C |
| | ATOM | 2496 | | RH | | -5.724 | 21.484 | 7.938 | 1.00 32.18 | | H | C |
| | MOTA | 2497 | | RH | | -5.415 | 22.610 | 8.716 | 1.00 28.43 | | H | C |
| | MOTA | 2498 | | RH | | -5.923 | 21.662 | 6.565 | 1.00 26.31 | | H | C |
| 20 | ATOM ATOM | 2499 2500 | | RH | | -5.306 -5.812 | 23.843 22.896 | 8.158 5.995 | 1.00 10.30 | | H | C |
| 20 | ATOM | 2501 | | RH | | -5.512 | 23.990 | 6.794 | 1.00 16.36 1.00 34.64 | | H H | C |
| | ATOM | 2502 | | RH | | -5.400 | 25.246 | 6.222 | 1.00 30.08 | | H | ŏ |
| | ATOM | 2503 | | PH | | -3.981 | 18.319 | 10.675 | 1.00 24.24 | | H | Ŋ |
| 05 | ATOM | 2504 | | PH | | -3.950 | 17.213 | 11.608 | 1.00 28.55 | | H | C |
| 25 | ATOM ATOM | 2505 2506 | | P H | | -4.657 -4.653 | 17.635 18.811 | 12.888 13.249 | 1.00 30.13 1.00 37.40 | | H | C |
| | MOTA | 2507 | | PH | | -2.504 | 16.839 | 13.249 11.947 | 1.00 37.40 | | H H | C |
| | ATOM | 2508 | | PH | | -1.662 | 16.413 | 10.790 | 1.00 25.38 | | H | Č |
| | MOTA | 2509 | | PH | | -1.428 | 17.107 | 9.634 | 1.00 18.65 | | H | С |
| 30 | ATOM | 2510 | | PH | | -0.956 | 15.178 | 10.665 | 1.00 30.58 | | H | C |
| | ATOM ATOM | 2511 2512 | | PH | | -0.630 -0.330 | 16.374 15.183 | 8.797 9.403 | 1.00 21.56 1.00 25.47 | | H | N |
| | ATOM | 2513 | | PH | | -0.796 | 14.065 | 11.495 | 1.00 28.45 | | H H | C |
| | ATOM | 2514 | | PH | | 0.436 | 14.123 | 8.956 | 1.00 15.55 | | H | C |
| 35 | MOTA | 2515 | | PH | | -0.027 | 13.003 | 11.044 | 1.00 24.57 | • | H | C |
| | MOTA | 2516 | | PH | | 0.574 | 13.039 | 9.786 | 1.00 26.41 | | H | C |
| | ATOM ATOM | 2517 2518 | | Y H | | -5.268 -5.920 | 16.677 16.993 | 13.573 14.825 | 1.00 30.49 | | H | N |
| | ATOM | 2519 | | YH | | -3.920 -4.886 | 16.815 | 15.917 | 1.00 23.23 1.00 24.33 | | H H | C |
| 40 | MOTA | 2520 | | ΥH | | -3.728 | 16.546 | 15.617 | 1.00 26.49 | | H | ŏ |
| | MOTA | 2521 | | NH | | -5.304 | 16.936 | 17.173 | 1.00 31.05 | | H | N |
| | MOTA | 2522 | | NH | | -4.403 | 16.809 | 18.313 | 1.00 30.94 | | H | C |
| | ATOM ATOM | 2523 2524 | | NH | | -4.074 -3.222 | 15.370 15.124 | 18.673 19.524 | 1.00 34.31 | | H | C |
| 45 | ATOM | 2525 | | NH | | -5.011 | 17.478 | 19.536 | 1.00 41.91 1.00 35.51 | | H H | C O |
| | ATOM | 2526 | | NH | | -6.191 | 18.384 | 19.228 | 1.00 52.15 | | H | Č |
| | MOTA | 2527 | | NH | | -7.414 | 18.042 | 20.070 | 1.00 68.67 | | H | C |
| | ATOM | 2528 | OE1 GL | | | -8.035 | 18.926 | 20.681 | 1.00 61.17 | | H | 0 |
| 50 | ATOM ATOM | 2529 2530 | NE2 GL N GL | X H | | -7.770 -4.755 | 16.752 14.420 | 20.105 18.051 | 1.00 55.73 1.00 32.59 | | H H | N |
| QU | ATOM | 2531 | | YH | | -4.490 | 13.026 | 18.354 | 1.00 32.33 | | H | C M |
| | ATOM | 2532 | C GL | ΥH | 106 | -5.137 | 12.508 | 19.633 | 1.00 28.80 | | H | č |
| | MOTA | 2533 | | ΥH | | -5.420 | 13.258 | 20.567 | 1.00 30.10 | | H | 0 |
| EE | ATOM | 2534 | | RH | | -5.384 | 11.209 | 19.668 | 1.00 29.41 | | H | Ŋ |
| 55 | ATOM ATOM | 2535 2536 | | R H R H | | -6.034 -5.319 | $10.448 \\ 9.124$ | 20.736 21.007 | 1.00 33.14 1.00 33.83 | | H H | C |
| | MOTA | 2537 | | RH | | -5.018 | 8.343 | 20.117 | 1.00 33.79 | | H | C O |
| | MOTA | 2538 | | RH | | -7.494 | 10.180 | 20.360 | 1.00 30.92 | | H | č |
| | MOTA | 2539 | | RH | | -8.205 | 9.778 | 21.533 | 1.00 42.28 | | H | 0 |
| 60 | MOTA | 2540 | | RH | | -7.572 | 9.043 | 19.335 | 1.00 32.35 | | H | C |
| | ATOM ATOM | 2541 2542 | | H U | | -5.026 -4.162 | 8.902 7.789 | 22.299 22.653 | 1.00 34.93 1.00 39.45 | | H H | И |
| | ATOM | 2543 | | UH | | -4.162 | 6.471 | 22.836 | 1.00 39.45 | | H H | C |
| | MOTA | 2544 | | UH | | -5.874 | 6.358 | 23.592 | 1.00 40.38 | | H | Ö |
| 65 | MOTA | 2545 | CB LE | H U | 108 | -3.419 | 8.155 | 23.936 | 1.00 39.65 | | H | C |
| | ATOM | 2546 | | UH | | -1.902 | 8.119 | 23.750 | 1.00 20.00 | | H | C |
| | ATOM ATOM | 2547 2548 | CD1 LE | | | -1.186 -1.292 | 9.177 6.767 | 24.596 24.127 | 1.00 20.00 1.00 20.00 | | H H | C |
| | MOTA | 2549 | | L H | | -4.448 | 5.462 | 22.077 | 1.00 20.00 | | H | N |
| | _ | | | - | | | · - | • • | | | - | |

| | ATOM ATOM | 2550 2551 2552 | CA C O | VAL H VAL H | 109 109 | -4.950 -3.831 -2.822 | 4.107 3.173 2.980 | 22.268 22.733 22.068 | 1.00 38.50 1.00 41.95 1.00 45.65 | Н Н Н | 0 C |
|----|--------------------------------------|--------------------------------------|-------------------------|----------------------------------|-------------------|--|--|--------------------------------------|--|------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM | 2553 2554 2555 2556 | CG2 N | VAL H VAL H VAL H ALA H | 109 109 110 | -5.504 -5.974 -6.670 -4.054 | 3.612 2.169 4.478 2.495 | 20.935 21.083 20.494 23.856 | 1.00 34.93 1.00 36.26 1.00 27.03 1.00 41.78 | н н н н | C C N |
| 10 | ATOM ATOM ATOM ATOM | 2557 2558 2559 2560 2561 | CA C O CB | ALA H ALA H ALA H | 110 110 110 | -3.117 -3.807 -4.881 -2.478 | 1.467 0.132 0.069 1.940 | 24.311 24.542 25.135 25.620 | 1.00 44.45 1.00 42.44 1.00 43.07 1.00 44.04 | н н н н | 0000 |
| 15 | ATOM ATOM ATOM ATOM ATOM | 2562 2563 2564 2565 | N CA C O CB | VAL H VAL H VAL H VAL H | 111 111 111 | -3.181 -3.591 -2.668 -1.552 -3.684 | -0.937 -2.301 -3.122 -3.511 | 24.070 24.195 25.091 24.737 | 1.00 43.71 1.00 46.41 1.00 48.72 1.00 51.00 | н н н н | N C O |
| 20 | ATOM ATOM ATOM ATOM | 2566 2567 2568 2569 | CG1 | VAL H VAL H SER H | 111 111 112 | -4.683 -4.189 -3.189 | -2.843 -3.970 -1.718 -3.346 | 22.793 22.741 21.897 26.316 | 1.00 46.04 1.00 52.67 1.00 36.76 1.00 53.18 | н н н | и С С |
| 20 | ATOM ATOM ATOM ATOM | 2570 2571 2572 2573 | CA C O CB | SER H SER H SER H SER H | 112 112 112 | -3.314 -4.756 -5.722 -2.838 -1.412 | -3.814 -4.215 -3.626 -2.698 -2.761 | 27.691 28.024 27.567 28.621 | 1.00 60.09 1.00 63.11 1.00 62.24 1.00 59.39 | н н н н | 0 0 0 |
| 25 | ATOM ATOM ATOM ATOM | 2574 2575 2576 2577 | N CA C | ALA H ALA H ALA H ALA H | 113 113 113 | -4.857 -3.631 -3.050 | -5.297 -5.952 -5.274 | 28.734 28.814 29.241 30.476 | 1.00 68.30 1.00 69.58 1.00 64.05 1.00 66.57 | н н н н | 0 N C |
| 30 | ATOM ATOM ATOM ATOM | 2578 2579 2580 2581 | O CB N CA C | ALA H ALA H ALA H ALA H | 113 114 114 | -1.951 -2.631 -3.851 -3.501 | -4.735 -5.866 -5.290 -4.512 | 30.471 28.085 31.555 32.735 | 1.00 67.66 1.00 61.17 1.00 74.52 1.00 75.18 | н н н н | O N C |
| 35 | ATOM ATOM ATOM | 2582 2583 2584 | O CB N | ALA H ALA H ALA H | 114 114 115 | -4.589 -5.200 -2.174 -4.843 | -3.481 -2.905 -3.801 -3.279 | 33.031 32.145 32.469 34.333 | 1.00 73.15 1.00 75.45 1.00 81.16 1.00 20.00 | н н н н | С О С И |
| 10 | ATOM ATOM ATOM ATOM | 2585 2586 2587 2588 | CA C O CB | ALA H ALA H ALA H ALA H | 115 115 115 | -5.951 -5.508 -4.381 -6.590 | -2.416 -0.977 -0.703 -3.008 | 34.716 34.986 35.374 35.973 | 1.00 20.00 1.00 20.00 1.00 20.00 1.00 20.00 | н н н н | C C C |
| 40 | ATOM ATOM ATOM ATOM | 2589 2590 2591 2592 | N CA C O | THR H THR H THR H THR H | 116 116 | -6.447 -6.197 -5.902 -6.514 | -0.042 1.360 1.553 0.955 | 34.728 35.045 36.534 37.408 | 1.00 48.17 1.00 49.91 1.00 53.54 1.00 61.76 | н н н н | И С О |
| 45 | ATOM ATOM ATOM ATOM | 2593 2594 2595 2596 | CB OG1 CG2 N | | 116 116 | -7.435 -8.157 -8.353 -4.893 | 2.174 2.541 1.345 2.401 | 34.652 35.832 33.753 36.803 | 1.00 51.97 1.00 59.75 1.00 67.33 1.00 55.71 | Н Н Н Н | И О С |
| 50 | ATOM ATOM ATOM | 2597 2598 2599 2600 | CA C O CB | THR H THR H THR H THR H | 117 117 117 | -4.516 -4.807 -4.390 -3.019 | 2.673 4.128 5.068 2.381 | 38.185 38.569 37.905 38.325 | 1.00 52.96 1.00 52.33 1.00 54.24 1.00 54.81 | Н Н Н | 0000 |
| 55 | ATOM ATOM ATOM ATOM ATOM | 2601 2602 2603 2604 | OG1 CG2 N CA | THR H PRO H PRO H | 117 118 118 | -2.778 -2.561 -5.242 -5.168 | 1.015 2.616 4.836 6.296 | 37.979 39.771 39.028 39.166 | 1.00 57.21 1.00 68.96 1.00 53.98 1.00 50.39 | H H H | C N |
| 60 | ATOM ATOM ATOM | 2605 2606 2607 2608 | C O CB CG | PRO H PRO H PRO H | 118 118 118 | -3.872 -3.247 -6.392 -6.424 | 6.738 5.971 6.611 5.452 | 39.851 40.578 40.004 40.935 | 1.00 51.76 1.00 52.75 1.00 53.07 1.00 53.57 | н н н н | 2000 |
| 60 | ATOM ATOM ATOM ATOM | 2609 2610 2611 2612 | CD N CA C | PRO H PRO H PRO H | 119 119 119 | -6.187 -3.460 -2.234 -2.362 | 4.277 7.992 8.518 9.092 | 40.010 39.634 40.231 41.640 | 1.00 56.15 1.00 50.77 1.00 51.99 1.00 57.32 | н н н н | C N C |
| 65 | ATOM ATOM ATOM ATOM | 2613 2614 2615 2616 | O CB CG CD | PRO H PRO H PRO H | 119 119 119 | -3.462 -1.824 -3.141 -3.998 | 9.238 9.590 10.178 8.943 | 42.177 39.237 38.879 38.645 | 1.00 60.85 1.00 47.61 1.00 45.24 1.00 53.33 | Н Н Н Н | 0000 |
| | ATOM ATOM | 2617 2618 | N CA | SER H SER H | | -1.206 -0.984 | 9.410 10.062 | 42.220 43.505 | 1.00 57.59 1.00 52.71 | H H | C |

| 5 | ATOM ATOM ATOM ATOM ATOM | 2619 2620 2621 2622 2623 | C O CB OG N | SER H 120 SER H 120 SER H 120 SER H 120 VAL H 121 | -(-(-1 |).150).994).264 L.175).788 | 11.331 11.313 9.075 8.049 12.470 | 43.342 42.911 44.427 44.829 43.667 | 1.00 50.89 1.00 55.25 1.00 56.41 1.00 63.45 1.00 48.38 | H H H H | [[[[| 0 0 0 |
|----|---|--|--------------------------------------|---|----------------|--|--|--|--|------------------|----------------------------|-------------|
| | MOTA MOTA MOTA MOTA | 2624 2625 2626 2627 | CA C O CB | VAL H 121 VAL H 121 VAL H 121 VAL H 121 | (~(~1 |).121).459).246 L.141 | 13.749 14.315 14.717 14.727 | 43.460 44.758 45.677 42.872 | 1.00 45.09 1.00 47.52 1.00 50.74 1.00 42.48 | F F F | I I I | 0000 |
| 10 | MOTA MOTA MOTA | 2628 2629 2630 2631 | CG1 CG2 N CA | VAL H 121 VAL H 121 TYR H 122 TYR H 122 | -2 | 0.418 2.052 1.803 2.482 | 15.856 14.002 14.298 14.867 | 42.140 41.898 44.822 45.978 | 1.00 41.61 1.00 38.28 1.00 48.88 1.00 46.62 | H H H | I I I | C N C |
| 15 | MOTA ATOM ATOM ATOM | 2632 2633 2634 2635 | C O CB CG | TYR H 122 TYR H 122 TYR H 122 TYR H 122 | | 3.043 3.566 3.622 3.084 | 16.256 16.512 13.924 12.561 | 45.663 44.587 46.372 46.632 | 1.00 49.87 1.00 52.32 1.00 42.13 1.00 39.14 | I | I I I | 0000 |
| 20 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 2636 2637 2638 2639 2640 2641 | CD1 CD2 CE1 CE2 CZ OH | TYR H 122 TYR H 122 TYR H 122 | | 2.084 3.566 1.560 3.049 2.055 | 12.381 11.462 11.118 10.197 10.022 8.763 | 47.583 45.921 47.816 46.160 47.106 47.359 | 1.00 33.27 1.00 26.44 1.00 39.62 1.00 41.31 1.00 39.35 1.00 46.83 |]]]] | I I I I I | CCCCCON |
| 25 | ATOM ATOM ATOM ATOM ATOM | 2642 2643 2644 2645 2646 | N CA C O CB | PRO H 123 PRO H 123 PRO H 123 PRO H 123 PRO H 123 | | 2.944 3.453 4.960 5.514 2.683 | 17.168 18.536 18.606 17.917 19.271 | 46.634 46.513 46.720 47.581 47.595 | 1.00 49.83 1.00 48.21 1.00 50.86 1.00 55.89 1.00 52.97 |]]] | H H H H | 0000 |
| 30 | ATOM ATOM ATOM ATOM | 2647 2648 2649 2650 | CG CD N CA | PRO H 123 PRO H 123 LEU H 124 LEU H 124 | | 2.564 2.201 5.626 7.066 7.407 | 18.226 16.986 19.432 19.575 20.984 | 48.667 47.893 45.923 46.038 46.455 | 1.00 51.62 1.00 43.80 1.00 49.83 1.00 52.27 1.00 48.73 | | H H H H H | C C C |
| 35 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 2651 2652 2653 2654 2655 2656 | | LEU H 124 LEU H 124 LEU H 124 LEU H 124 LEU H 124 LEU H 124 | | 7.380 7.767 7.671 8.332 8.326 | 21.915 19.224 17.772 17.628 16.840 | 45.648 44.715 44.212 42.853 45.212 | 1.00 48.20 1.00 56.15 1.00 53.01 1.00 48.39 1.00 59.89 | | H H H H H | 00000 |
| 40 | ATOM ATOM ATOM ATOM ATOM | 2657 2658 2659 2660 2661 | N CA C O CB | ALA H 125 ALA H 125 ALA H 125 ALA H 125 ALA H 125 | | 7.717 8.080 9.551 0.094 7.241 | 21.118 22.389 22.353 21.295 22.631 | 47.739 48.337 48.710 49.017 49.580 | 1.00 50.01 1.00 52.85 1.00 54.62 1.00 52.85 1.00 58.29 | | H H H H H | и С С |
| 45 | ATOM ATOM ATOM ATOM | 2662 2663 2664 2665 | N CA C O | PRO H 126 PRO H 126 PRO H 126 PRO H 126 | 1 1 1 | 0.221 1.639 1.834 0.808 | 23.514 23.574 23.154 23.018 25.040 | 48.676 49.027 50.475 51.175 48.803 | 1.00 53.35 1.00 54.53 1.00 56.27 1.00 61.53 1.00 53.66 | | H H H H H | и С С |
| 50 | ATOM ATOM ATOM ATOM ATOM | 2666 2667 2668 2669 2670 | N | PRO H 126 PRO H 126 PRO H 126 PRO H 126 THR H 132 | 1 1 1 | 9.705 12.997 16.845 | 25.727 24.858 22.974 30.323 30.845 | 49.091 48.370 50.894 49.326 48.416 | 1.00 60.53 1.00 48.22 1.00 62.11 1.00131.55 1.00132.47 | | H H H H H | 0 0 0 |
| 55 | ATOM ATOM ATOM ATOM ATOM | 2671 2672 2673 2674 2675 | CA C O CB OG3 | | 1 1 3 | L6.091 L5.683 L4.472 L4.446 | 32.322 33.228 30.679 31.461 | 48.094 48.815 49.089 50.283 | 1.00130.65 1.00132.15 1.00132.60 1.00134.97 | | H H H H H | 0000 |
| 60 | MOTA ATOM ATOM MOTA MOTA | 2676 2677 2678 2679 2680 | CG2 N CA C O | ASN H 133 ASN H 133 ASN H 133 ASN H 133 ASN H 133 | | L4.250 L6.828 L7.281 L7.045 L7.646 | 29.214 32.548 33.902 34.267 33.716 | 49.466 46.981 46.666 45.195 44.283 | 1.00131.87 1.00126.17 1.00123.00 1.00118.12 1.00118.63 | | H H H H | И С С |
| 65 | MOTA MOTA MOTA MOTA MOTA MOTA MOTA MOTA | 2681 2682 2683 2684 2685 2686 2687 | CB CG OD: | ASN H 133 ASN H 133 1 ASN H 133 2 ASN H 133 SER H 134 SER H 134 SER H 134 | | 18.787 19.063 18.749 19.650 16.086 15.901 | 33.958 34.983 34.801 36.111 35.203 35.788 35.123 | 46.968 48.039 49.212 47.602 44.979 43.649 42.828 | | | H H H H H H | ССОИИСС |
| | 114 014 | _00, | _ | | | | | | | | | |

| | n m∪M | 2688 | 0 | SER H 134 | 14.092 | 35.767 | 42.048 | 1.00 96.71 | Н | 0 |
|----|--------------|---------------------|-----------|--------------------------|------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM ATOM | 2689 | CB | SER H 134 | 17.225 | 35.729 | 42.888 | 1.00102.40 | H | č |
| | ATOM | 2690 | ŌĞ | SER H 134 | 17.391 | 36.936 | 42.142 | 1.00 92.26 | H | 0 |
| | ATOM | 2691 | N | MET H 135 | 14.681 | 33.758 | 42.950 | 1.00 85.97 | H | N |
| 5 | MOTA | 2692 | CA | MET H 135 | 13.640 | 33.007 | 42.214 | 1.00 75.45 | H | C |
| | MOTA | 2693 | C | MET H 135 | 13.234 | 31.737 | 42.977 | 1.00 68.66 | H | C |
| | MOTA | 2694 | 0 | MET H 135 | 13.837 | 31.393 | 44.037 | 1.00 67.11 | H H | 0 |
| | ATOM | 2695 2696 | CB | MET H 135 MET H 135 | 14.158 13.679 | 32.619 33.454 | 40.827 39.620 | 1.00 78.16 1.00 87.38 | п Н | C |
| 10 | MOTA MOTA | 2697 | CG SD | MET H 135 | 11.912 | 33.393 | 39.425 | 1.00 37.33 | H | S |
| 10 | ATOM | 2698 | CE | MET H 135 | 11.764 | 33.473 | 37.638 | 1.00 95.09 | H | č |
| | MOTA | 2699 | N | VAL H 136 | 12.396 | 30.924 | 42.576 | 1.00 66.53 | H | N |
| | ATOM | 2700 | CA | VAL H 136 | 11.862 | 29.787 | 43.312 | 1.00 64.38 | H | С |
| | MOTA | 2701 | C | VAL H 136 | 11.450 | 28.655 | 42.383 | 1.00 60.86 | H | C |
| 15 | ATOM | 2702 | 0 | VAL H 136 | 10.794 | 28.881 | 41.369 | 1.00 60.52 | H | 0 |
| | MOTA | 2703 | CB | VAL H 136 | 10.649 | 30.194 | 44.185 | 1.00 63.71 | H | C |
| | MOTA | 2704 | | VAL H 136 | 10.017 11.092 | 28.972 31.164 | 44.813 45.262 | 1.00 66.52 1.00 70.97 | H H | G G |
| | MOTA MOTA | 2705 2706 | N N | VAL H 136 THR H 137 | 11.032 | 27.444 | 42.607 | 1.00 70.37 | H | N |
| 20 | ATOM | 2707 | CA | THR H 137 | 11.265 | 26.333 | 41.842 | 1.00 55.89 | H | Ĉ |
| _0 | ATOM | 2708 | C | THR H 137 | 10.464 | 25.399 | 42.735 | 1.00 52.85 | H | С |
| | ATOM | 2709 | 0 | THR H 137 | 10.980 | 24.867 | 43.714 | 1.00 51.83 | H | 0 |
| | MOTA | 2710 | CB | THR H 137 | 12.358 | 25.492 | 41.165 | 1.00 54.09 | H | C |
| | MOTA | 2711 | OG1 | | 12.942 | 26.229 | 40.087 | 1.00 48.58 | H | 0 |
| 25 | MOTA | 2712 | CG2 | THR H 137 LEU H 138 | 11.772 9.195 | 24.201 25.219 | 40.637 42.404 | 1.00 57.49 1.00 50.91 | H H | N C |
| | ATOM ATOM | 2713 2714 | CA | LEU H 138 | 8.350 | 24.318 | 43.162 | 1.00 51.88 | H | Č |
| | MOTA | 2715 | C | LEU H 138 | 8.027 | 23.184 | 42.220 | 1.00 49.95 | H | č |
| | ATOM | 2716 | ō | LEU H 138 | 8.260 | 23.294 | 41.012 | 1.00 53.08 | H | 0 |
| 30 | MOTA | 2717 | CB | LEU H 138 | 7.071 | 25.016 | 43.622 | 1.00 50.53 | H | C |
| | MOTA | 2718 | CG | LEU H 138 | 7.313 | 26.155 | 44.613 | 1.00 46.88 | H | C |
| | MOTA | 2719 | | LEU H 138 | 5.996 | 26.848 | 44.934 | 1.00 62.88 | H | C |
| | ATOM | 2720 | | CLY H 138 | 7.944 7.498 | 25.611 22.091 | 45.870 42.753 | 1.00 75.29 1.00 47.47 | H H | C N |
| 35 | ATOM ATOM | 2721 2722 | N CA | GLY H 139 | 7.197 | 20.974 | 41.887 | 1.00 46.51 | Н | C |
| 33 | ATOM | 2723 | C | GLY H 139 | 5.959 | 20.195 | 42.244 | 1.00 47.53 | H | Ċ |
| | ATOM | 2724 | ŏ | GLY H 139 | 5.297 | 20.467 | 43.235 | 1.00 48.18 | H | 0 |
| | MOTA | 2725 | N | CYS H 140 | 5.663 | 19.205 | 41.414 | 1.00 52.13 | H | N |
| | MOTA | 2726 | CA | CYS H 140 | 4.503 | 18.351 | 41.592 | 1.00 54.83 | H | C |
| 40 | ATOM | 2727 | C | CYS H 140 | 4.940 | 16.925 | 41.247 | 1.00 49.40 | H | C |
| | MOTA MOTA | 2728 2729 | O CB | CYS H 140 CYS H 140 | 5.633 3.377 | 16.698 18.813 | 40.250 40.655 | 1.00 44.99 1.00 57.10 | H H | 0 |
| | ATOM | 2730 | SG | CYS H 140 | 1.704 | 18.276 | 41.141 | 1.00 76.47 | H | s |
| | ATOM | 2731 | N | LEU H 141 | 4.548 | 15.969 | 42.081 | 1.00 46.30 | H | N |
| 45 | MOTA | 2732 | CA | LEU H 141 | 4.910 | 14.580 | 41.850 | 1.00 42.12 | H | C |
| | MOTA | 2733 | ď | LEU H 141 | 3.646 | 13.734 | 41.662 | 1.00 40.17 | H | G |
| | ATOM | 2734 | 0_ | LEU H 141 | 2.882 | 13.523 | 42.601 | 1.00 39.80 1.00 46.51 | H | 0 |
| | MOTA | 2735 2736 | CB CG | LEU H 141 LEU H 141 | 5.735 6.288 | 14.055 12.631 | 43.031 42.945 | 1.00 46.51 | H H | C |
| 50 | MOTA MOTA | 2737 | | LEU H 141 | 7.259 | 12.570 | 41.784 | 1.00 55.61 | H | Ğ |
| 00 | ATOM | 2738 | | LEU H 141 | 7.002 | 12.237 | 44.232 | 1.00 52.23 | H | Ċ |
| | MOTA | 2739 | N | VAL H 142 | 3.440 | 13.268 | 40.432 | 1.00 38.37 | H | N |
| | MOTA | 2740 | CA | VAL H 142 | 2.291 | 12.450 | 40.068 | 1.00 37.81 | H | C |
| | MOTA | 2741 | C | VAL H 142 | 2.758 | 10.999 | 39.994 | 1.00 43.46 | H | C |
| 55 | ATOM | 2742 | 0 | VAL H 142 | 3.168 | 10.522 | 38.935 | 1.00 44.35 | H H | 0 |
| | MOTA | $\frac{2743}{2744}$ | CB CC1 | VAL H 142 L VAL H 142 | 1.729 0.661 | 12.889 11.913 | 38.695 38.221 | 1.00 37.90 1.00 34.13 | H | C |
| | MOTA MOTA | 2745 | | 2 VAL H 142 | 1.149 | 14.283 | 38.799 | 1.00 29.37 | H | č |
| | MOTA | 2746 | N | LYS H 143 | 2.684 | 10.292 | 41.118 | 1.00 45.16 | H | N |
| 60 | MOTA | 2747 | CA | LYS H 143 | 3.163 | 8.920 | 41.167 | 1.00 41.48 | H | C |
| | MOTA | 2748 | C | LYS H 143 | 2.141 | 7.798 | 40.999 | 1.00 46.30 | H | C |
| | ATOM | 2749 | 0 | LYS H 143 | 1.027 | 7.834 | 41.549 | 1.00 45.34 | H | 0 |
| | MOTA | 2750 | CB | LYS H 143 | 3.939 | 8.711 | 42.467 | 1.00 43.20 | H H | C |
| 6F | MOTA MOTA | 2751 2752 | CG CD | LYS H 143 LYS H 143 | 4.963 5.743 | 7.582 7.500 | 42.413 43.720 | 1.00 41.99 1.00 42.24 | H H | G G |
| 65 | ATOM | 2753 | CE | LYS H 143 | 6.993 | 6.653 | 43.720 | 1.00 52.65 | H | č |
| | MOTA | 2754 | NZ | LYS H 143 | 6.693 | 5.280 | 43.090 | 1.00 67.31 | H | Ň |
| | MOTA | 2755 | N | GLY H 144 | 2.549 | 6.791 | 40.233 | 1.00 47.62 | H | N |
| | ATOM | 2756 | CA | GLY H 144 | 1.704 | 5.640 | 39.988 | 1.00 52.58 | H | С |

| | "ATOM | 2757 | С | GLY H | 1/1/ | 0.369 | 5.882 | 39.299 | 1.00 55.82 | Н | C |
|----|-------|------|--------------|-------|------|--------|--------|--------|------------|---|-----|
| | | | | | | | | | | | - |
| | MOTA | 2758 | 0 | GLY H | | -0.560 | 6.422 | 39.890 | 1.00 63.65 | H | _ |
| | MOTA | 2759 | \mathbf{N} | TYR H | 145 | 0.283 | 5.482 | 38.037 | 1.00 52.96 | H | N |
| | ATOM | 2760 | ca | TYR H | 145 | -0.942 | 5.599 | 37.259 | 1.00 46.96 | H | C |
| 5 | MOTA | 2761 | С | TYR H | 145 | -0.820 | 4.849 | 35.930 | 1.00 44.52 | H | C |
| | MOTA | 2762 | 0 | TYR H | 145 | 0.277 | 4.623 | 35.418 | 1.00 43.14 | H | |
| | MOTA | 2763 | СB | TYR H | | -1.302 | 7.062 | 37.002 | 1.00 41.24 | H | |
| | ATOM | 2764 | CG | TYR H | | -0.336 | 7.807 | 36.121 | 1.00 54.18 | H | |
| | | | | | | | | | | | |
| | MOTA | 2765 | CD1 | | | 0.721 | 8.522 | 36.670 | 1.00 52.12 | H | |
| 10 | MOTA | 2766 | CD2 | TYR H | | -0.501 | 7.827 | 34.740 | 1.00 37.28 | H | |
| | MOTA | 2767 | | TYR H | 145 | 1.586 | 9.246 | 35.871 | 1.00 48.23 | H | |
| | MOTA | 2768 | CE2 | TYR H | 145 | 0.358 | 8.543 | 33.934 | 1.00 45.82 | H | C |
| | MOTA | 2769 | CZ | TYR H | 145 | 1.399 | 9.258 | 34.506 | 1.00 53.37 | H | |
| | MOTA | 2770 | OH | TYR H | | 2.232 | 10.020 | 33.716 | 1.00 51.96 | н | |
| 15 | ATOM | 2771 | N | PHE H | | -1.963 | 4.454 | 35.385 | 1.00 47.52 | H | |
| 13 | | 2772 | | | 146 | -2.002 | 3.718 | 34.133 | 1.00 40.66 | H | |
| | MOTA | | CA | | | | | | | | |
| | MOTA | 2773 | C | PHE H | | -3.418 | 3.793 | 33.579 | 1.00 38.13 | H | |
| | MOTA | 2774 | 0 | PHE H | | -4.387 | 3.717 | 34.324 | 1.00 37.80 | H | |
| | MOTA | 2775 | CB | PHE H | | -1.600 | 2.266 | 34.387 | 1.00 32.65 | H | |
| 20 | MOTA | 2776 | CG | PHE H | 146 | -1.391 | 1.468 | 33.139 | 1.00 40.82 | H | C |
| | MOTA | 2777 | CD1 | PHE H | 146 | -2.463 | 0.908 | 32.463 | 1.00 41.99 | H | |
| | ATOM | 2778 | CD2 | | | -0.119 | 1.288 | 32.625 | 1.00 38.82 | H | |
| | MOTA | 2779 | | PHE H | | -2.266 | 0.188 | 31.305 | 1.00 39.34 | H | |
| | MOTA | 2780 | CE2 | | | 0.080 | 0.567 | 31.460 | 1.00 32.29 | H | |
| 05 | | | | | | | | | | | |
| 25 | ATOM | 2781 | CZ | PHE H | | -0.995 | 0.019 | 30.804 | 1.00 28.82 | H | |
| | ATOM | 2782 | N | PRO H | | -3.554 | 3.994 | 32.262 | 1.00 41.70 | H | |
| | MOTA | 2783 | CA | PRO H | | -2.444 | 4.151 | 31.325 | 1.00 39.65 | H | |
| | MOTA | 2784 | C | PRO H | 147 | -2.207 | 5.630 | 31.123 | 1.00 41.99 | H | C |
| | MOTA | 2785 | 0 | PRO H | 147 | -2.689 | 6.456 | 31.898 | 1.00 39.17 | H | . 0 |
| 30 | ATOM | 2786 | CB | PRO H | 147 | -2.986 | 3.507 | 30.068 | 1.00 41.33 | н | |
| | MOTA | 2787 | ĊĠ | PRO H | | -4.403 | 4.014 | 30.077 | 1.00 36.45 | H | |
| | | 2788 | CD | PRO H | | -4.829 | 3.857 | 31.530 | 1.00 45.61 | H | |
| | ATOM | | | | | | | | | | |
| | ATOM | 2789 | N | GLU H | | -1.459 | 5.961 | 30.080 | 1.00 40.49 | H | |
| | MOTA | 2790 | $^{\rm CA}$ | GLU H | | -1.200 | 7.352 | 29.770 | 1.00 42.77 | H | _ |
| 35 | MOTA | 2791 | С | GLU H | | -2.481 | 7.814 | 29.103 | 1.00 48.73 | H | |
| | MOTA | 2792 | 0 | GLU H | 148 | -3.292 | 6.993 | 28.683 | 1.00 56.82 | H | . 0 |
| | ATOM | 2793 | CB | GLU H | 148 | -0.021 | 7.464 | 28.809 | 1.00 41.73 | H | С |
| | MOTA | 2794 | CG | GLU H | 148 | 1.342 | 7.286 | 29.473 | 1.00 44.10 | H | C |
| | ATOM | 2795 | CD | GLU H | | 1.914 | 8.593 | 30.018 | 1.00 54.54 | H | |
| 40 | ATOM | 2796 | OE1 | | | 1.268 | 9.240 | 30.872 | 1.00 49.74 | H | |
| 40 | ATOM | 2797 | OE2 | | | 3.021 | 8.977 | 29.584 | 1.00 48.09 | H | |
| | | | | | | | | | | | |
| | ATOM | 2798 | N | PRO H | | -2.698 | 9.131 | 29.018 | 1.00 48.93 | H | |
| | MOTA | 2799 | CA | PRO H | | -1.771 | 10.127 | 29.533 | 1.00 46.06 | H | |
| | ATOM | 2800 | С | PRO H | | -2.349 | 10.712 | 30.808 | 1.00 46.54 | H | |
| 45 | ATOM | 2801 | 0 | PRO H | 149 | -3.262 | 10.155 | 31.410 | 1.00 52.02 | H | |
| | MOTA | 2802 | CB | PRO H | 149 | -1.760 | 11.148 | 28.424 | 1.00 47.59 | H | C |
| | MOTA | 2803 | CG | PRO H | 149 | -3.227 | 11.241 | 28.133 | 1.00 35.29 | H | C |
| | ATOM | 2804 | CD | PRO H | | -3.673 | 9.775 | 28.118 | 1.00 46,53 | H | |
| | MOTA | 2805 | N | VAL H | | -1.797 | 11.845 | 31.199 | 1.00 46.48 | H | |
| 50 | ATOM | 2806 | CA | VAL H | | -2.239 | 12.617 | 32.336 | 1.00 48.36 | H | |
| JU | | | | | | | | | | | |
| | ATOM | 2807 | C | VAL H | | -1.769 | 13.975 | 31.976 | 1.00 51.53 | H | |
| | ATOM | 2808 | 0 | VAL H | | -0.866 | 14.111 | 31.166 | 1.00 49.48 | H | |
| | ATOM | 2809 | CB | VAL H | | -1.528 | 12.172 | 33.638 | 1.00 46.55 | H | |
| | MOTA | 2810 | CG1 | VAL H | 150 | -2.023 | 10.810 | 34.129 | 1.00 52.35 | H | C |
| 55 | ATOM | 2811 | CG2 | VAL H | 150 | -0.022 | 12.133 | 33.442 | 1.00 45.34 | H | C |
| | MOTA | 2812 | N | THR H | | -2.457 | 14.985 | 32.493 | 1.00 53.87 | H | |
| | ATOM | 2813 | CA | THR H | | -2.050 | 16.343 | 32.179 | 1.00 52.79 | H | |
| | MOTA | 2814 | C | THR H | | -1.853 | 17.094 | 33.467 | 1.00 53.87 | H | |
| | | | | | | -2.467 | | 34.480 | | H | |
| 00 | MOTA | 2815 | 0 | THR H | | | 16.801 | | 1.00 58.71 | | |
| 60 | MOTA | 2816 | CB | THR H | | -3.167 | 17.041 | 31.389 | 1.00 49.68 | H | |
| | MOTA | 2817 | | THR H | | -4.169 | 17.497 | 32.300 | 1.00 68.43 | H | |
| | ATOM | 2818 | CG2 | THR H | 151 | -3.814 | 16.082 | 30.390 | 1.00 50.57 | H | |
| | MOTA | 2819 | N | VAL H | | -0.916 | 18.052 | 33.417 | 1.00 54.84 | H | |
| | MOTA | 2820 | CA | VAL H | | -0.653 | 18.890 | 34.576 | 1.00 52.95 | H | |
| 65 | ATOM | 2821 | C | VAL H | | -0.556 | 20.338 | 34.132 | 1.00 52.63 | H | |
| | ATOM | 2822 | Ö | VAL H | | 0.044 | 20.670 | 33.121 | 1.00 50.48 | H | |
| | ATOM | 2823 | | VAL H | | 0.672 | 18.465 | 35.236 | 1.00 51.86 | H | |
| | | | CB CC1 | | | | | | 1.00 31.86 | | |
| | MOTA | 2824 | | VAL H | | 0.613 | 17.013 | 35.714 | | | |
| | MOTA | 2825 | CG2 | VAL H | T27 | 1.840 | 18.631 | 34.275 | 1.00 53.57 | H | C |

| | ATOM ATOM ATOM | 2826 2827 2828 | N CA C | THR H THR H THR H | 153 | -1.249. -1.215 -0.947 | 21.203 22.630 23.377 | 34.887 34.594 35.880 | 1.00 53.77 1.00 56.85 1.00 59.60 | H | I C |
|-----|----------------------|----------------------|--------------|-------------------------|------|-----------------------------|----------------------------|----------------------------|--|--------|-----|
| | ATOM | 2829 | ŏ | THR H | | -1.146 | 22.862 | 36.971 | 1.00 59.00 | H H | _ |
| 5 | MOTA | 2830 | CB | THR H | | -2.589 | 23.061 | 34.048 | 1.00 58.09 | H | |
| * | ATOM | 2831 | | THR H | | -3.610 | 22.721 | 34.987 | 1.00 63.79 | H | _ |
| | ATOM ATOM | 2832 2833 | CG2 N | THR H | | -2.889 -0.428 | 22.371 24.607 | 32.711 | 1.00 53.38 | F | |
| | ATOM | 2834 | CA | | 154 | -0.428 | 25.388 | 35.743 36.943 | 1.00 58.56 1.00 59.00 | H H | |
| 10 | ATOM | 2835 | C | | 154 | -1.058 | 26.617 | 36.985 | 1.00 65.51 | H | |
| | ATOM | 2836 | 0 | TRP H | | -1.090 | 27.437 | 36.077 | 1.00 68.44 | I: | |
| | MOTA | 2837 | CB | TRP H | | 1.310 | 25.839 | 36.936 | 1.00 58.83 | H | |
| | ATOM ATOM | 2838 2839 | CG CD1 | TRP H | | 2.220 | 24.700 23.892 | 37.226 | 1.00 63.23 | H | - |
| 15 | ATOM | 2840 | CD1 | | 154 | 2.867 2.606 | 23.892 | 36.276 38.526 | 1.00 63.79 1.00 55.01 | H H | |
| , , | ATOM | 2841 | NE1 | | | 3.610 | 22.909 | 36.827 | 1.00 52.78 | H | |
| | MOTA | 2842 | CE2 | | | 3.457 | 23.068 | 38.283 | 1.00 53.67 | H | |
| | ATOM | 2843 | CE3 | | | 2.315 | 24.533 | 39.802 | 1.00 48.82 | H | |
| 20 | ATOM ATOM | 2844 2845 | CZ2 CZ3 | | | 3.988 2.848 | 22.352 23.811 | 39.320 40.856 | 1.00 47.95 1.00 41.43 | H | |
| | ATOM | 2846 | | TRP H | | 3.692 | 22.703 | 40.610 | 1.00 41.43 | H | |
| | ATOM | 2847 | N | ASN H | | -1.843 | 26.698 | 38.075 | 1.00 67.18 | H | |
| | ATOM | 2848 | CA | ASN H | | -2.816 | 27.773 | 38.189 | 1.00 70.56 | H | C |
| 25 | ATOM ATOM | 2849 2850 | C O | ASN H ASN H | | -3.788 | 27.780 | 37.006 | 1.00 69.10 | H | |
| 2.0 | ATOM | 2851 | CB | ASN H | | -4.096 -2.065 | 28.808 29.103 | 36.419 38.255 | 1.00 71.27 1.00 70.76 | H H | |
| | ATOM | 2852 | CG | ASN H | | -1.537 | 29.314 | 39.652 | 1.00 70.70 | H | |
| | MOTA | 2853 | | ASN H | 155 | -2.077 | 28.814 | 40.634 | 1.00 71.53 | H | |
| 00 | ATOM | 2854 | | ASN H | | -0.448 | 30.098 | 39.732 | 1.00 64.39 | H | |
| 30 | ATOM ATOM | 2855 2856 | N CA | SER H SER H | | -4.242 -5.245 | 26.570 26.483 | 36.631 35.576 | 1.00 71.92 1.00 71.41 | H | - |
| | ATOM | 2857 | C | SER H | | -4.670 | 26.875 | 34.212 | 1.00 71.41 | H H | _ |
| | ATOM | 2858 | Ō | SER H | | -5.371 | 26.975 | 33.212 | 1.00 74.08 | H | |
| | ATOM | 2859 | CB | SER H | | -6.398 | 27.417 | 35.949 | 1.00 74.57 | Н | |
| 35 | MOTA | 2860 | OG | SER H | | -6.915 | 27.040 | 37.226 | 1.00 75.73 | Н | _ |
| | ATOM ATOM | 2861 2862 | N CA | GLY H | | -3.349 -2.698 | 27.138 27.495 | 34.201 32.944 | 1.00 69.68 1.00 67.44 | H H | |
| | ATOM | 2863 | C | GLY H | | -2.203 | 28.945 | 32.952 | 1.00 70.86 | H | |
| | ATOM | 2864 | 0 | GLY H | | -1.597 | 29.433 | 32.006 | 1.00 67.86 | H | |
| 40 | ATOM | 2865 | N | SER H | | -2.527 | 29.647 | 34.058 | 1.00 74.60 | H | - |
| | ATOM ATOM | 2866 2867 | CA C | SER H SER H | | -2.075 -0.548 | 31.029 31.120 | 34.216 34.273 | 1.00 82.23 1.00 82.78 | H | - |
| | ATOM | 2868 | Ö | SER H | | 0.060 | 32.135 | 33.958 | 1.00 82.78 1.00 85.81 | H H | - |
| | ATOM | 2869 | CB | SER H | | -2.678 | 31.578 | 35.513 | 1.00 83.01 | H | |
| 45 | ATOM | 2870 | OG | SER H | | -2.040 | 30.961 | 36.632 | 1.00 99.77 | H | |
| | ATOM ATOM | 2871 2872 | N CA | LEU H LEU H | | 0.069 1.525 | 30.015 | 34.734 | 1.00 82.52 | H | |
| | ATOM | 2873 | CA | LEU H | | 2.021 | 29.954 29.704 | 34.677 33.252 | 1.00 82.36 1.00 86.99 | H H | - |
| | ATOM | 2874 | ŏ | LEU H | 159 | 2.025 | 28.590 | 32.747 | 1.00 79.57 | H | |
| 50 | ATOM | 2875 | CB | LEU H | | 1.993 | 28.822 | 35.593 | 1.00 81.28 | H | С |
| | MOTA MOTA | 2876 2877 | CG CD1 | LEU H | | 1.795 | 29.147 | 37.075 | 1.00 79.39 | H | |
| | ATOM | 2878 | | LEU H | | 2.518 2.313 | 28.155 30.535 | 37.989 37.455 | 1.00 93.68 1.00 62.45 | H H | |
| | ATOM | 2879 | N | SER H | | 2.414 | 30.808 | 32.585 | 1.00 02.43 | H | |
| 55 | ATOM | 2880 | CA | SER H | 160 | 2.816 | 30.704 | 31.185 | 1.00 96.23 | H | |
| | ATOM | 2881 | C | SER H | | 3.963 | 29.706 | 31.006 | 1.00 92.96 | H | C |
| | ATOM ATOM | 2882 2883 | O CB | SER H SER H | | 3.782 3.255 | 28.495 32.089 | 30.993 | 1.00 88.20 1.00102.14 | H | |
| | ATOM | 2884 | OG | SER H | | 3.409 | 32.948 | 30.707 31.837 | 1.00102.14 | H H | |
| 60 | ATOM | 2885 | N | SER H | 161 | 5.176 | 30.264 | 30.814 | 1.00 89.77 | H | |
| | MOTA | 2886 | CA | SER H | 161 | 6.356 | 29.411 | 30.734 | 1.00 86.56 | H | C |
| | ATOM | 2887 | C | SER H | | 7.054 | 29.317 | 32.093 | 1.00 77.91 | H | |
| | ATOM ATOM | 2888 2889 | O CB | SER H SER H | | 6.63 <u>4</u> 7.309 | 29.900 30.008 | 33.083 29.700 | 1.00 71.05 1.00 92.32 | H | |
| 65 | ATOM | 2890 | OG | SER H | | 7.193 | 29.283 | 28.475 | 1.00 92.32 | H H | |
| | MOTA | 2891 | N | GLY H | 162 | 8.133 | 28.513 | 32.130 | 1.00 69.90 | н | |
| | ATOM | 2892 | CA | GLY H | | 8.873 | 28.369 | 33.379 | 1.00 63.56 | H | С |
| | ATOM ATOM | 2893 2894 | C O | GLY H | | 8.509 9.024 | 27.071 | 34.104 | 1.00 59.46 | H | |
| | AT ON | 40J 4 | J | ם זות | 4.02 | J.U44 | 26.747 | 35.165 | 1.00 61.58 | H | 0 |

| | ATOM | 2895 | N | VAL H | 163 | 7.550 | 26.337 | 33.511 | 1.00 56.46 | F | ı N | |
|----|------|------|-------------|-------|-----|--------|--------|--------|------------|---|-----|---|
| | MOTA | 2896 | CA | VAL H | | 7.159 | 25.060 | 34.093 | 1.00 51.91 | | I C | |
| | MOTA | 2897 | C | VAL H | | 7.695 | 23.886 | 33.267 | 1.00 46.10 | | ı c | |
| | ATOM | 2898 | õ | VAL H | | 7.597 | 23.847 | 32.048 | 1.00 54.99 | | - 0 | |
| 5 | MOTA | 2899 | ČВ | VAL H | | 5.632 | 25.007 | 34.142 | 1.00 56.36 | | ı c | |
| 3 | MOTA | 2900 | | VAL H | | 5.049 | 26.077 | 33.222 | 1.00 41.84 | | i C | |
| | | 2901 | | VAL H | | 5.145 | 23.641 | 33.693 | 1.00 37.01 | | - | |
| | MOTA | | | | | | | | 1.00 37.01 | | - | |
| | ATOM | 2902 | N | HIS H | | 8.321 | 22.926 | 33.973 | | | I N | |
| | MOTA | 2903 | CA | HIS H | | 8.861 | 21.764 | 33.277 | 1.00 38.20 | | I C | |
| 10 | MOTA | 2904 | C | HIS H | | 8.049 | 20.502 | 33.578 | 1.00 39.02 | | H C | |
| | ATOM | 2905 | 0 | HIS H | | 7.976 | 20.032 | 34.706 | 1.00 45.91 | | O I | |
| | MOTA | 2906 | CB | HIS H | | 10.313 | 21.577 | 33.717 | 1.00 47.41 | | H C | |
| | MOTA | 2907 | CG | HIS H | | 11.186 | 22.595 | 33.029 | 1.00 50.39 | | H C | |
| | MOTA | 2908 | ND1 | HIS H | 164 | 11.185 | 22.791 | 31.687 | 1.00 44.32 | I | I | |
| 15 | ATOM | 2909 | CD2 | HIS H | 164 | 12.121 | 23.462 | 33.604 | 1.00 55.52 | I | H C | |
| | MOTA | 2910 | | HIS H | | 12.100 | 23.754 | 31.461 | 1.00 48.81 | F | H C | |
| | MOTA | 2911 | NE2 | HIS H | 164 | 12.675 | 24.174 | 32.590 | 1.00 54.09 | I | H N | |
| | MOTA | 2912 | N | THR H | 165 | 7.370 | 19.928 | 32.580 | 1.00 38.94 | I | H N | |
| | MOTA | 2913 | ca | THR H | 165 | 6.670 | 18.686 | 32.816 | 1.00 34.58 | I | H C | |
| 20 | MOTA | 2914 | C | THR H | | 7.399 | 17.560 | 32.128 | 1.00 34.70 | I | H C | |
| | ATOM | 2915 | Õ | THR H | | 7.479 | 17.480 | 30.909 | 1.00 36.98 | | O E | |
| | ATOM | 2916 | ČВ | THR H | | 5.254 | 18.805 | 32.243 | 1.00 29.54 | | H C | |
| | MOTA | 2917 | OG1 | | | 4.542 | 19.815 | 32.962 | 1.00 26.80 | | O | |
| | MOTA | 2918 | CG2 | | | 4.511 | 17.466 | 32.408 | 1.00 30.37 | | H C | |
| 25 | ATOM | 2919 | N | PHE H | | 8.006 | 16.715 | 32.970 | 1.00 33.46 | | i N | |
| 20 | ATOM | 2920 | CA | PHE H | | 8.843 | 15.652 | 32.438 | 1.00 30.02 | | H C | |
| | ATOM | 2921 | C | PHE H | | 8.045 | 14.422 | 32.045 | 1.00 34.42 | | H C | |
| | | 2922 | 0 | PHE H | | 7.017 | 14.068 | 32.608 | 1.00 34.42 | | | |
| | ATOM | 2923 | | PHE H | | 9.859 | 15.259 | 33.516 | 1.00 30.92 | | | |
| 20 | ATOM | | CB | | | 10.715 | 16.432 | 33.877 | 1.00 30.92 | | | |
| 30 | ATOM | 2924 | CG | PHE H | | | | | | | H C | |
| | ATOM | 2925 | | PHE H | | 11.915 | 16.636 | 33.210 | 1.00 29.02 | | H C | |
| | MOTA | 2926 | | PHE H | | 10.295 | 17.316 | 34.855 | 1.00 31.79 | | H C | |
| | ATOM | 2927 | | PHE H | | 12.682 | 17.749 | 33.512 | 1.00 31.45 | | H C | |
| | MOTA | 2928 | CE2 | | | 11.072 | 18.429 | 35.148 | 1.00 24.79 | | H C | |
| 35 | MOTA | 2929 | $^{\rm CZ}$ | PHE H | | 12.266 | 18.654 | 34.478 | 1.00 30.14 | | H C | |
| | MOTA | 2930 | N | PRO H | | 8.539 | 13.777 | 31.009 | 1.00 39.29 | | H N | |
| | MOTA | 2931 | $^{\rm CA}$ | PRO H | | 7.977 | 12.558 | 30.445 | 1.00 42.13 | | H C | |
| | MOTA | 2932 | С | PRO H | | 7.936 | 11.450 | 31.506 | 1.00 47.73 | | H C | |
| | MOTA | 2933 | 0 | PRO H | 167 | 8.821 | 11.347 | 32.335 | 1.00 56.66 | I | O E | |
| 40 | ATOM | 2934 | CB | PRO H | 167 | 8.910 | 12.175 | 29.309 | 1.00 45.03 | I | H C | |
| | MOTA | 2935 | ÇG | PRO H | 167 | 9.508 | 13.500 | 28.826 | 1.00 46.59 | I | H C | |
| | MOTA | 2936 | CD | PRO H | 167 | 9.720 | 14.174 | 30.268 | 1.00 34.51 |] | H C | , |
| | MOTA | 2937 | N | ALA H | 168 | 6.837 | 10.656 | 31.518 | 1.00 45.33 | I | H N | i |
| | ATOM | 2938 | CA | ALA H | 168 | 6.700 | 9.658 | 32.569 | 1.00 42.85 | I | H C | , |
| 45 | ATOM | 2939 | С | ALA H | 168 | 7.589 | 8.447 | 32.291 | 1.00 42.34 | 1 | H C | |
| | MOTA | 2940 | Ó | ALA H | | 7.978 | 8.165 | 31.165 | 1.00 39.56 |] | O F | |
| | ATOM | 2941 | | ALA H | | 5.236 | 9.220 | 32.623 | 1.00 37.42 | I | H C | |
| | ATOM | 2942 | N | VAL H | | 7.951 | 7.746 | 33.381 | 1.00 41.75 | | H N | |
| | ATOM | 2943 | CA | VAL H | | 8.708 | 6.508 | 33.239 | 1.00 41.72 | | H C | |
| 50 | MOTA | 2944 | CB | VAL H | | 9.960 | 6.609 | 34.111 | 1.00 45.04 | | H Č | |
| • | ATOM | 2945 | | VAL H | | 10.743 | 5.299 | 34.055 | 1.00 58.27 | | H C | |
| | MOTA | 2946 | | VAL H | | 10.845 | 7.742 | 33.624 | 1.00 43.30 | | i Č | |
| | MOTA | 2947 | 0 | VAL H | | 7.107 | 5.322 | 34.609 | 1.00 47.89 | | O E | |
| | MOTA | 2948 | N | LEU H | | 8.029 | 4.209 | 32.879 | 1.00 47.24 | | H N | |
| 55 | | 2949 | CA | LEU H | | 7.293 | 2.994 | 33.196 | 1.00 47.57 | | H C | |
| 55 | MOTA | | | LEU H | | | | | 1.00 47.57 | | | |
| | MOTA | 2950 | C | | | 8.099 | 2.072 | 34.110 | | | | |
| | ATOM | 2951 | O | LEU H | | 9.213 | 1.663 | 33.813 | 1.00 53.71 | | O E | |
| | ATOM | 2952 | CB | LEU H | | 6.966 | 2.273 | 31.889 | 1.00 49.56 | | H C | |
| | MOTA | 2953 | CG | LEU H | | 5.944 | 1.151 | 32.084 | 1.00 43.50 | | H C | |
| 60 | MOTA | 2954 | | LEU H | | 4.717 | 1.614 | 32.875 | 1.00 47.61 | | H C | |
| | MOTA | 2955 | | LEU H | | 5.417 | 0.594 | 30.761 | 1.00 40.91 | | H C | |
| | ATOM | 2956 | N | GLU H | | 7.509 | 1.787 | 35.285 | 1.00 55.65 | | H N | |
| | MOTA | 2957 | CA | GLU H | | 8.159 | 0.876 | 36.217 | 1.00 68.14 | | H C | |
| _ | MOTA | 2958 | С | GLU H | | 7.197 | -0.226 | 36.666 | 1.00 67.74 | | H C | |
| 65 | ATOM | 2959 | 0 | GLU H | | 6.098 | 0.029 | 37.140 | 1.00 65.41 | | O F | |
| | ATOM | 2960 | CB | GLU H | | 8.626 | 1.686 | 37.428 | 1.00 72.43 | | H C | |
| | MOTA | 2961 | CG | GLU H | | 9.934 | 1.159 | 38.021 | 1.00 91.59 | | H C | |
| | MOTA | 2962 | $^{\rm CD}$ | GLU H | | 10.146 | 1.768 | 39.388 | 1.00120.67 | | H C | |
| | MOTA | 2963 | OE1 | GLU H | 171 | 11.228 | 1.613 | 39.940 | 1.00130.29 | 1 | O E | ŀ |
| | | | | | | | | | | | | |

| | MOTA | 2964 | | GLU H | | | .216 | 2.391 | 39.899 | 1.00122.92 | H | 0 |
|----|------|-------|-------------|-------|-------|----|-------|--------|--------|------------|---|---|
| | ATOM | 2965 | N | SER H | | | .611 | -1.486 | 36.449 | 1.00 72.50 | H | N |
| | MOTA | 2966 | CA | SER H | | | .698 | -2.576 | 36.764 | 1.00 78.89 | H | C |
| | ATOM | .2967 | C | SER H | 172 | 5 | .564 | -2.629 | 35.737 | 1.00 79.78 | H | С |
| 5 | MOTA | 2968 | 0 | SER H | 172 | 5 | .392 | -3.582 | 34.986 | 1,00 87,21 | H | 0 |
| | ATOM | 2969 | CB | SER H | 172 | 6 | .099 | -2.293 | 38,141 | 1,00 79,72 | H | C |
| | MOTA | 2970 | OG | SER H | 172 | | .766 | -1.804 | 37.968 | 1.00 80.07 | H | ō |
| | ATOM | 2971 | N | ASP H | | | .739 | -1.563 | 35.781 | 1.00 74.99 | H | N |
| | ATOM | 2972 | CA | ASP H | | | .654 | -1.391 | 34.824 | | | |
| 10 | | 2973 | | | | | | | | 1.00 72.78 | H | C |
| 10 | ATOM | | C | ASP H | | | .866 | -0.123 | 35.157 | 1.00 65.42 | H | C |
| | ATOM | 2974 | 0_ | ASP H | | | .678 | 0.008 | 34.893 | 1.00 59.35 | H | 0 |
| | MOTA | 2975 | CB | ASP H | | | .748 | -2.625 | 34.859 | 1.00 81.69 | H | С |
| | ATOM | 2976 | CG | ASP H | 173 | 2 | .371 | -3.008 | 33.430 | 1.00 97.36 | H | С |
| | ATOM | 2977 | OD1 | ASP H | 173 | 2 | .070 | -2.099 | 32.654 | 1.00108.23 | H | 0 |
| 15 | ATOM | 2978 | OD2 | ASP H | 173 | 2 | .357 | -4.193 | 33,120 | 1,00106.64 | H | Ō |
| | ATOM | 2979 | N | LEU H | 174 | | .586 | 0.813 | 35.796 | 1.00 63.54 | H | Ň |
| | ATOM | 2980 | CA | LEU H | | | .969 | 2.059 | 36.232 | 1.00 55.65 | H | Ç |
| | ATOM | 2981 | C | LEU H | | | .798 | 3.286 | 35.812 | 1.00 51.40 | | |
| | ATOM | 2982 | | LEU H | | | | | | | H | C |
| 00 | | | O | | | | .019 | 3.255 | 35.734 | 1.00 54.33 | H | 0 |
| 20 | ATOM | 2983 | CB | LEU H | | | .819 | 2.014 | 37.760 | 1.00 54.66 | H | C |
| | MOTA | 2984 | CG | LEU H | | | .767 | 0.993 | 38.222 | 1.00 48.08 | H | С |
| | ATOM | 2985 | | LEU H | | | .941 | 0.589 | 39.689 | 1.00 53.16 | H | C |
| | MOTA | 2986 | CD2 | LEU H | | 0 | .335 | 1.512 | 38.091 | 1.00 59.23 | H | C |
| | ATOM | 2987 | N | TYR H | 175 | 3 | .150 | 4.419 | 35.548 | 1.00 43.17 | H | N |
| 25 | MOTA | 2988 | CA | TYR H | 175 | 3 | .870 | 5.631 | 35.150 | 1.00 41.68 | H | C |
| | ATOM | 2989 | C | TYR H | | | .025 | 6.621 | 36.287 | 1.00 40.74 | H | č |
| | ATOM | 2990 | ŏ | TYR H | | | .233 | 6.637 | 37.226 | 1.00 36.93 | H | ŏ |
| | ATOM | 2991 | СВ | TYR H | | | .156 | 6.354 | 33.997 | | | |
| | | | | | | | | | | 1.00 47.72 | H | C |
| 00 | ATOM | 2992 | CG | TYR H | | | .166 | 5.631 | 32.667 | 1.00 53.98 | H | C |
| 30 | MOTA | 2993 | | TYR H | | | .346 | 5.452 | 31.955 | 1.00 51.27 | H | C |
| | ATOM | 2994 | CD2 | | | | .992 | 5.105 | 32.137 | 1.00 47.22 | H | С |
| | MOTA | 2995 | CE1 | TYR H | 175 | 4 | .354 | 4.764 | 30.754 | 1.00 58.28 | H | С |
| | ATOM | 2996 | CE2 | TYR H | 175 | 1 | .992 | 4.418 | 30.948 | 1.00 54.50 | H | C |
| | MOTA | 2997 | CZ | TYR H | 175 | 3 | .171 | 4.243 | 30.257 | 1.00 55.81 | Н | Ċ |
| 35 | ATOM | 2998 | OH | TYR H | | | .166 | 3.509 | 29.089 | 1.00 41.75 | H | ŏ |
| - | ATOM | 2999 | N | THR H | | | .058 | 7.452 | 36.171 | 1.00 41.73 | H | |
| | ATOM | 3000 | | THR H | | | .362 | | | | | N |
| | | | CA | | | | | 8.499 | 37.139 | 1.00 38.73 | H | C |
| | ATOM | 3001 | C | THR H | | | .921 | 9.671 | 36.350 | 1.00 41.82 | H | C |
| | ATOM | 3002 | 0 | THR H | | | .933 | 9.528 | 35.645 | 1.00 36.33 | H | 0 |
| 40 | ATOM | 3003 | $^{\rm CB}$ | THR H | | | .468 | 8.094 | 38.131 | 1.00 41.02 | H | C |
| | MOTA | 3004 | OG1 | THR H | 176 | 6. | .251 | 6.754 | 38.592 | 1.00 49.99 | H | 0 |
| | MOTA | 3005 | CG2 | THR H | 176 | 6 | .480 | 9.045 | 39.310 | 1.00 36.35 | H | C |
| | MOTA | 3006 | N | LEU H | 177 | 5 | .268 | 10.822 | 36.439 | 1.00 38.99 | Н | N |
| | ATOM | 3007 | CA | LEU H | 177 | | .783 | 11.982 | 35.743 | 1.00 33.71 | H | C |
| 45 | ATOM | 3008 | C | LEU H | | | .070 | 12.988 | 36.820 | 1.00 32.17 | H | č |
| | ATOM | 3009 | ŏ | LEU H | | | .689 | 12.796 | 37.962 | 1.00 32.19 | H | ŏ |
| | ATOM | 3010 | СВ | LEU H | | | .779 | 12.526 | 34.729 | 1.00 30.29 | | |
| | | | | | | | | | | | H | C |
| | MOTA | 3011 | CG | LEU H | 177 | | .660 | 13.499 | 35.078 | 1.00 31.11 | H | C |
| | ATOM | 3012 | CDI | LEU H | T / / | | .186 | 14.867 | 35.498 | 1.00 32.05 | H | C |
| 50 | ATOM | 3013 | | LEU H | | | .830 | 13.652 | 33.831 | 1.00 37.80 | H | С |
| | ATOM | 3014 | N | SER H | | | .751 | 14.060 | 36.463 | 1.00 37.29 | H | N |
| | MOTA | 3015 | CA | SER H | 178 | 7. | .105 | 15.065 | 37.440 | 1.00 36.26 | H | C |
| | ATOM | 3016 | C | SER H | 178 | 6. | .994 | 16.416 | 36.761 | 1.00 40.62 | H | C |
| | MOTA | 3017 | 0 | SER H | | | .258 | 16.532 | 35.562 | 1.00 37.73 | H | ō |
| 55 | ATOM | 3018 | СВ | SER H | | | .534 | 14.831 | 37.906 | 1.00 33.83 | H | Č |
| - | ATOM | 3019 | OG | SER H | | | .654 | | | | | |
| | | 3020 | | | | | | 15.142 | 39.273 | 1.00 53.70 | H | 0 |
| | ATOM | | N | SER H | | | .600 | 17.437 | 37.511 | 1.00 35.74 | H | N |
| | ATOM | 3021 | CA | SER H | | | .437 | 18.737 | 36.871 | 1.00 36.88 | H | C |
| | MOTA | 3022 | C | SER H | | | .953 | 19.862 | 37.767 | 1.00 39.97 | H | C |
| 60 | ATOM | 3023 | 0 | SER H | | | .677 | 19.929 | 38.957 | 1.00 43.93 | H | 0 |
| | ATOM | 3024 | CB | SER H | 179 | 4. | .951 | 18.948 | 36.573 | 1.00 41.66 | H | C |
| | ATOM | 3025 | OG | SER H | | | .812 | 19.938 | 35.551 | 1.00 41.44 | H | ō |
| | MOTA | 3026 | N | SER H | | | .770 | 20.740 | 37.161 | 1.00 44.77 | H | И |
| | ATOM | 3027 | ČA | SER H | | | .376 | 21.808 | 37.101 | 1.00 47.17 | H | |
| 65 | ATOM | 3028 | C | SER H | | | .933 | 23.189 | 37.460 | 1.00 47.17 | | C |
| 33 | | 3028 | | | | | | | | | H | C |
| | MOTA | | O | SER H | | | .776 | 23.451 | 36.275 | 1.00 56.63 | H | 0 |
| | ATOM | 3030 | CB | SER H | | | . 893 | 21.679 | 37.813 | 1.00 46.70 | H | C |
| | ATOM | 3031 | OG | SER H | | | 300 | 22.191 | 36.544 | 1.00 39.66 | H | 0 |
| | ATOM | 3032 | N | H LAV | 181 | 7. | .692 | 24.080 | 38.438 | 1.00 54.79 | H | N |

| | ATOM ATOM ATOM | 3033 3034 3035 | CA C O | VAL H 1 VAL H 1 | 181 181 | 7.318 8.212 8.466 | 26.458 26.375 | 38.796 39.990 | 1.00 50.47 | H H | I C |
|----|------------------------------|------------------------------|---------------------|--|-------------------|------------------------------------|--------------------------------------|--------------------------------------|--|------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM | 3036 3037 3038 3039 | CG N | 1 VAL H 1 2 VAL H 1 THR H 1 | 181 181 182 | 5.862 5.748 5.365 8.750 | 25.673 26.985 | 40.024 37.951 | 1.00 47.12 1.00 39.28 | H H H | 1 C |
| 10 | ATOM ATOM ATOM ATOM | 3040 3041 3042 3043 | CA C O CB | THR H 1 THR H 1 | L82 L82 | 9.638 8.954 8.259 10.948 | 28.427 29.788 30.134 28.523 | 38.599 38.586 37.629 | 1.00 48.08 1.00 51.63 | H H H | 1 C |
| 15 | ATOM ATOM ATOM ATOM | 3044 3045 3046 3047 | | 1 THR H 1 2 THR H 1 VAL H 1 | 182 182 183 | 11.621 11.855 9.161 | 27.264 29.590 30.555 | 37.831 38.363 39.653 | 1.00 51.81 1.00 29.17 1.00 56.66 | H H H | C N |
| | MOTA MOTA MOTA | 3048 3049 3050 | С О СВ | VAL H 1 VAL H 1 VAL H 1 | .83 .83 .83 | 8.566 9.449 10.231 7.199 | 31.882 32.755 32.257 31.834 | 39.791 40.650 41.454 40.508 | 1.00 57.17 1.00 59.90 1.00 59.55 1.00 58.93 | н н н н | CO |
| 20 | ATOM ATOM ATOM ATOM | 3051 3052 3053 3054 | | 1 VAL H 1 2 VAL H 1 PRO H 1 PRO H 1 | .83 .84 | 6.271 7.403 9.329 10.142 | 30.839 31.475 34.080 34.990 | 39.826 41.971 40.496 41.300 | 1.00 61.72 1.00 41.35 1.00 66.40 1.00 66.49 | н н н | C C N |
| 25 | MOTA MOTA MOTA MOTA | 3055 3056 3057 3058 | C O CB CG | PRO H 1 PRO H 1 PRO H 1 | .84 .84 .84 | 9.825 8.738 9.673 | 34.725 34.249 36.367 | 42.765 43.093 40.841 | 1.00 67.25 1.00 66.00 1.00 64.64 | н н н н | C O |
| | ATOM MOTA MOTA | 3059 3060 3061 | CD N CA | PRO H 1 PRO H 1 SER H 1 SER H 1 | 84 85 | 9.314 8.552 10.779 10.586 | 36.132 34.825 35.012 34.790 | 39.408 39.491 43.640 45.061 | 1.00 71.49 1.00 70.81 1.00 66.78 1.00 67.40 | н н н | N C C |
| 30 | ATOM ATOM ATOM ATOM | 3062 3063 3064 | C O CB | SER H 1 SER H 1 SER H 1 | 85 85 | 9.352 8.673 11.827 | 35.537 35.081 35.245 | 45.572 46.492 45.817 | 1.00 72.49 1.00 73.45 1.00 66.63 | н н н н | C 0 |
| 35 | ATOM ATOM ATOM | 3065 3066 3067 3068 | OG N CA C | SER H 1 SER H 1 SER H 1 SER H 1 | 86 86 | 12.993 9.061 7.904 6.633 | 34.763 36.689 37.461 36.611 | 45.181 44.977 45.399 45.310 | 1.00 65.52 1.00 72.88 1.00 76.17 | н н н | C N O |
| 40 | ATOM ATOM ATOM | 3069 3070 3071 | O CB OG | SER H 1 SER H 1 SER H 1 | 86 86 86 | 6.016 7.768 8.710 | 36.312 38.737 38.758 | 46.336 44.554 43.495 | 1.00 78.37 1.00 80.30 1.00 75.54 1.00 64.86 | н н н н | 0000 |
| 40 | ATOM ATOM ATOM ATOM | 3072 3073 3074 3075 | N CA C O | PRO H 18 PRO H 18 PRO H 18 PRO H 18 | 87 87 | 6.246 5.051 4.756 | 36.185 35.367 34.323 | 44.089 43.859 44.928 | 1.00 75.34 1.00 69.64 1.00 66.91 | Н Н Н | N C C |
| 45 | ATOM ATOM ATOM | 3076 3077 3078 | CB CG CD | PRO H 18 PRO H 18 PRO H 18 | 87 87 | 3.648 5.332 6.029 6.996 | 34.269 34.736 35.838 36.358 | 45.451 42.502 41.782 42.829 | 1.00 68.67 1.00 71.74 1.00 71.69 1.00 78.09 | н н н н | 0 0 0 |
| 50 | MOTA MOTA ATOM ATOM | 3079 3080 3081 3082 | N CA C | ARG H 18 ARG H 18 ARG H 18 | 88 88 | 5.745 5.568 6.649 | 33.496 32.446 32.600 | 45.251 46.255 47.319 | 1.00 65.41 1.00 66.06 1.00 71.72 | H H H | C N |
| 00 | ATOM ATOM ATOM | 3082 3083 3084 3085 | CB CB CD | ARG H 18 ARG H 18 ARG H 18 ARG H 18 | 38 38 | 7.776 5.680 4.610 4.956 | 32.982 31.070 30.050 29.292 | 47.017 45.583 45.956 47.212 | 1.00 73.68 1.00 63.16 1.00 47.34 | H H H | С С |
| 55 | ATOM ATOM ATOM | 3086 3087 3088 | NE CZ NH1 | ARG H 18 ARG H 18 ARG H 18 | 38 38 38 | 6.371 6.941 6.221 | 28.942 28.200 27.717 | 47.242 48.185 49.188 | 1.00 42.91 1.00 58.37 1.00 63.59 1.00 58.02 | H H H H | С И С И |
| 60 | ATOM ATOM ATOM ATOM | 3089 3090 3091 3092 | NH2 N CA C | ARG H 18 PRO H 18 PRO H 18 PRO H 18 | 39 39 | 8.239 6.324 5.021 | 27.947 32.290 31.810 | 48.132 48.581 49.055 | 1.00 75.00 1.00 73.56 1.00 76.25 | H H H | N N C |
| | ATOM ATOM ATOM | 3093 3094 3095 | O CB CG | PRO H 18 PRO H 18 PRO H 18 | 39 39 | 4.006 3.307 5.400 6.524 | 32.893 32.775 30.964 31.757 | 49.415 50.421 50.263 50.848 | 1.00 80.21 1.00 86.41 1.00 76.00 1.00 75.53 | Н Н Н Н | 0 0 0 |
| 65 | ATOM ATOM ATOM | 3097 3098 | CD N CA | PRO H 18 SER H 19 SER H 19 | 39 90 90 | 7.346 3.915 2.963 | 32.143 33.940 35.010 | 49.633 48.603 48.879 | 1.00 74.81 1.00 80.77 1.00 82.18 | H H H | С С С |
| | ATOM ATOM ATOM | 3100 | C O CB | SER H 19 SER H 19 SER H 19 | 0 | 1.719 0.702 3.578 | 34.817 35.464 36.377 | 48.030 48.254 48.571 | 1.00 81.86 1.00 81.36 1.00 83.27 | Н Н Н | C C |

| | ATOM | 3102 | OG | SER H | 190 | 3.707 | 36.570 | 47.174 | 1.00 87.49 | , | Ħ | 0 |
|----|--------------|--------------|-----------|----------------|-----|------------------|------------------|------------------|--------------------------|---|---|--------|
| | ATOM | 3102 | N | GLU H | | 1.811 | 33.924 | 47.052 | 1.00 81.18 | | | N |
| | ATOM | 3104 | CA | GLU H | | 0.694 | 33.642 | 46.162 | 1.00 80.63 | | | C |
| | ATOM | 3105 | C | GLU H | | 0.523 | 32.143 | 45.934 | 1.00 82.13 | | | č |
| 5 | MOTA | 3106 | ō | GLU H | | 1.465 | 31.447 | 45.558 | 1.00 80.46 | 3 | | 0 |
| | ATOM | 3107 | СВ | GLU H | 191 | 0.903 | 34.334 | 44.820 | 1.00 81.67 | 3 | | С |
| | MOTA | 3108 | CG | GLU H | | 0.887 | 35.844 | 44.879 | 1.00 78.66 | | | С |
| | ATOM | 3109 | CD | GLU H | | 1.138 | 36.466 | 43.518 | 1.00 84.10 | | | C |
| | MOTA | 3110 | OE1 | | | 0.440 | 36.081 | 42.552 | 1.00 79.16 | | | 0 |
| 10 | ATOM | 3111 | OE2 | GLU H | | 2.028 | 37.338 | 43.417 | 1.00 84.64 | | | 0 |
| | MOTA | 3112 | N | THR H | | -0.697 -1.035 | 31.665 30.254 | 46.150 45.998 | 1.00 82.97 1.00 82.00 | | | Ŋ |
| | ATOM ATOM | 3113 3114 | CA C | THR H | | -0.683 | 29.609 | 44.663 | 1.00 82.00 | | | C C |
| | MOTA | 3115 | Ö | THR H | | -1.405 | 29.767 | 43.679 | 1.00 80.71 | | | Ö |
| 15 | ATOM | 3116 | СВ | THR H | | -2.536 | 30.021 | 46.230 | 1.00 80.05 | | | Č |
| | ATOM | 3117 | OG1 | | | -2.869 | 30.370 | 47.577 | 1.00 88.12 | | | Ō |
| | MOTA | 3118 | CG2 | THR H | 192 | -2.895 | 28.569 | 45.978 | 1.00 78.28 | ; | H | C |
| | MOTA | 3119 | N | VAL H | | 0.426 | 28.877 | 44.636 | 1.00 75.98 | | | N |
| | ATOM | 3120 | CA | VAL H | | 0.836 | 28.165 | 43.432 | 1.00 68.25 | | | Č |
| 20 | MOTA | 3121 | C | VAL H | | 0.149 | 26.807 | 43.529 | 1.00 65.36 | | | C |
| | MOTA | 3122 | 0 | VAL H | | 0.328 2.360 | 26.087 27.972 | 44.509 43.384 | 1.00 64.64 1.00 66.83 | | | С О |
| | ATOM ATOM | 3123 3124 | CB CC1 | VAL H VAL H | | 2.718 | 27.022 | 42.265 | 1.00 70.86 | | | C |
| | ATOM | 3125 | | VAL H | | 3.046 | 29.313 | 43.170 | 1.00 66.13 | | | C |
| 25 | MOTA | 3126 | N | THR H | | -0.644 | 26.455 | 42.525 | 1.00 64.29 | | | N |
| | ATOM | 3127 | CA | THR H | | -1.364 | 25.190 | 42.575 | 1.00 65.18 | | | C |
| | MOTA | 3128 | C | THR H | 194 | -1.173 | 24.250 | 41.390 | 1.00 63.54 | | | C |
| | MOTA | 3129 | 0 | THR H | | -1.145 | 24.670 | 40.237 | 1.00 64.27 | | | 0 |
| | MOTA | 3130 | CB | THR H | | -2.869 | 25.437 | 42.752 | 1.00 65.84 | | | C |
| 30 | ATOM | 3131 | OG1 | | | -3.085 | 26.186 | 43.952 | 1.00 67.51 | | | 0 |
| | MOTA | 3132 3133 | CG2 | THR H | | -3.622 -1.068 | 24.110 22.964 | 42.825 41.702 | 1.00 67.60 1.00 60.79 | | | N |
| | ATOM ATOM | 3134 | N CA | CYS H | | -0.878 | 21.930 | 40.699 | 1.00 61.12 | | | Ç. |
| | ATOM | 3135 | C | CYS H | | -2.215 | 21.268 | 40.365 | 1.00 57.72 | | | Č |
| 35 | ATOM | 3136 | ŏ | CYS H | | -2.912 | 20.771 | 41.248 | 1.00 56.12 | | | ŏ |
| | MOTA | 3137 | CB | CYS H | | 0.124 | 20.891 | 41.222 | 1.00 60.88 | | | C |
| | ATOM | 3138 | SG | CYS H | | 0.445 | 19.499 | 40.098 | 1.00 74.47 | | H | S |
| | MOTA | 3139 | N | ASN H | | -2.559 | 21.265 | 39.081 | 1.00 52.67 | | | N |
| | MOTA | 3140 | CA | ASN H | | -3.807 | 20.682 | 38.606 | 1.00 53.59 | | | C |
| 40 | MOTA | 3141 | C | ASN H | | -3.467 | 19.433 | 37.787 | 1.00 52.35 1.00 51.73 | | | C |
| | MOTA MOTA | 3142 3143 | O CB | ASN H ASN H | | -2.757 -4.535 | 19.523 21.701 | 36.785 37.728 | 1.00 51.73 | | | 0 |
| | MOTA | 3144 | CG | ASN H | | -4.395 | 23.130 | 38.247 | 1.00 62.00 | | | C |
| | MOTA | 3145 | OD1 | | | -4.161 | 24.061 | 37.472 | 1.00 67.81 | | | ŏ |
| 45 | MOTA | 3146 | | ASN H | | -4.541 | 23.310 | 39.556 | 1.00 65.11 | | H | N |
| | MOTA | 3147 | N | VAL H | | -3.982 | 18.276 | 38.199 | 1.00 49.58 | | H | N |
| | MOTA | 3148 | CA | VAL H | | -3.689 | 17.016 | 37.512 | 1.00 46.57 | | H | C |
| | ATOM | 3149 | C | VAL H | | -4.930 | 16.190 | 37.159 | 1.00 48.56 | | | Č |
| E0 | MOTA | 3150 3151 | 0 | H JAV | | -5.888 -2.750 | 16.135 16.143 | 37.925 38.381 | 1.00 53.48 1.00 44.48 | | | C |
| 50 | MOTA MOTA | 3152 | CB | VAL H VAL H | | -2.750 -2.412 | 14.851 | 37.666 | 1.00 39.07 | | | C |
| | MOTA | 3153 | | VAL H | | -1.495 | 16.923 | 38.718 | 1.00 37.49 | | H | Č |
| | ATOM | 3154 | N | ALA H | | -4.897 | 15.532 | 36.002 | 1.00 49.52 | | | N |
| | ATOM | 3155 | CA | ALA H | | -6.021 | 14.717 | 35.551 | 1.00 48.53 | | | C |
| 55 | ATOM | 3156 | C | ALA H | | -5.610 | 13.434 | 34.832 | 1.00 51.07 | | | C |
| | MOTA | 3157 | 0 | ALA H | | -4.711 | 13.441 | 33.993 | 1.00 55.91 | | | 0 |
| | MOTA | 3158 | СВ | ALA H | | -6.910 | 15.543 | 34.643 | 1.00 48.57 | | | C |
| | MOTA | 3159 | N | HIS H | | -6.281 | 12.336 | 35.174 | 1.00 54.83 1.00 51.27 | | | N |
| 60 | MOTA MOTA | 3160 3161 | CA C | HIS H | | -6.037 -7.384 | 11.031 10.385 | 34.561 34.250 | 1.00 51.27 | | | G G |
| 00 | ATOM | 3162 | Ö | HIS H | | -7.882 | 9.555 | 35.002 | 1.00 46.18 | | | Ö |
| | ATOM | 3163 | СВ | HIS H | | -5.218 | 10.138 | 35.496 | 1.00 47.91 | | | č |
| | MOTA | 3164 | CG | HIS H | | -5.003 | 8.745 | 34.982 | 1.00 42.99 | | | Č |
| | MOTA | 3165 | | HIS H | | -5.849 | 7.699 | 35.281 | 1.00 52.90 | | H | N |
| 65 | MOTA | 3166 | | HIS H | | -4.026 | 8.221 | 34.203 | 1.00 52.68 | | | C |
| | MOTA | 3167 | CE1 | HIS H | 199 | -5.403 | 6.593 | 34.713 | 1.00 50.68 | | | C |
| | MOTA | 3168 | | HIS H | | -4.297 | 6.882 | 34.053 | 1.00 47.65 | | | N |
| | ATOM | 3169 | N | PRO H | | -7.989 -9.277 | 10.778 10.323 | 33.120 32.593 | 1.00 58.59 1.00 60.75 | | | C |
| | MOTA | 3170 | CA | PRO H | ∠∪∪ | -9.277 | 10.343 | 24.333 | T.00 00.75 | | | _ |

| | a | | | | | | | | | | |
|---------|------|------|------------------|---------|-----|---------|---------|---------|------------|---|-----|
| | ATOM | 3171 | С | PRO H | 200 | -9.504 | 8.822 | 32.689 | 1.00 60.27 | Н | С |
| | | | | | | | | | | | |
| | MOTA | 3172 | 0 | PRO H | | ~10.551 | 8.376 | 33.152 | 1.00 64.21 | H | 0 |
| | MOTA | 3173 | CB | PRO H | 200 | -9.236 | 10.800 | 31.146 | 1.00 61.93 | H | C |
| | ATOM | 3174 | CG | PRO H | 200 | -8.483 | 12.082 | 31.255 | 1.00 60.39 | H | C |
| | | | | | | | | | | | |
| 5 | MOTA | 3175 | $^{\rm CD}$ | PRO H | | -7.342 | 11.699 | 32.167 | 1.00 60.10 | H | C |
| | MOTA | 3176 | \mathbf{N} | ALA H | 201 | -8.523 | 8.047 | 32.244 | 1.00 57.28 | H | N |
| | MOTA | 3177 | CA | ALA H | 201 | -8.632 | 6.600 | 32.269 | 1.00 57.95 | H | C |
| | | | | | | | | | - | | |
| | ATOM | 3178 | C | ALA H | | -9.267 | 6.127 | 33.578 | 1.00 64.27 | H | C |
| | ATOM | 3179 | 0 | ALA H | 201 | -9.869 | 5.054 | 33.641 | 1.00 67.28 | H | 0 |
| 10 | MOTA | 3180 | CB | ALA H | 201 | -7.263 | 5.979 | 32.079 | 1.00 53.21 | H | С |
| 10 | | 3181 | | SER H | | -9.135 | 6.936 | 34.620 | 1.00 64.03 | H | Ŋ |
| | MOTA | | N | | | | | | | | |
| | MOTA | 3182 | ca | SER H | 202 | -9.708 | 6.603 | 35.912 | 1.00 67.56 | H | C |
| | MOTA | 3183 | C | SER H | 202 | ~10.529 | 7.790 | 36.400 | 1.00 71.63 | H | C |
| | MOTA | 3184 | Õ | SER H | | -11.048 | 7.783 | 37.516 | 1.00 75.10 | H | · Ö |
| | | | | | | | | | | | |
| 15 | ATOM | 3185 | $^{\mathrm{CB}}$ | SER H | | -8.602 | 6.301 | 36.919 | 1.00 68.02 | H | С |
| | MOTA | 3186 | OG | SER H | 202 | -7.878 | 7.475 | 37.234 | 1.00 60.70 | H | 0 |
| | MOTA | 3187 | N | SER H | | -10.639 | 8.809 | 35.552 | 1.00 73.88 | H | N |
| | | | | | | | | | | | |
| | ATOM | 3188 | ca | SER H | | -11.383 | 10.014 | 35.887 | 1.00 75.67 | H | Ċ |
| | ATOM | 3189 | C | SER H | 203 | -10.951 | 10.512 | 37.253 | 1.00 70.02 | H | С |
| 20 | MOTA | 3190 | 0 | SER H | 203 | -11.738 | 10.537 | 38.190 | 1.00 70.12 | H | 0 |
| 20 | | | | | | | | 35.888 | | | |
| | MOTA | 3191 | CB | SER H | | -12.888 | 9.732 | | 1.00 81.76 | H | C |
| | ATOM | 3192 | OG | SER H | 203 | -13.367 | 9.502 | 34.571 | 1.00 92.44 | H | 0 |
| | MOTA | 3193 | N | THR H | 204 | -9.690 | 10.908 | 37.353 | 1.00 69.13 | H | N |
| | MOTA | 3194 | CA | THR H | | -9.129 | 11.395 | 38.602 | 1.00 68.07 | H | Ċ |
| | | | | | | | | | | | |
| 25 | MOTA | 3195 | C | THR H | | -8.638 | 12.825 | 38.462 | 1.00 69.60 | H | C |
| | MOTA | 3196 | 0 | THR H | 204 | -7.549 | 13.069 | 37.955 | 1.00 75.93 | H | 0 |
| | ATOM | 3197 | СB | THR H | | -7.941 | 10.523 | 39.038 | 1.00 67.90 | H | C |
| | | | | | | | | | | | |
| | MOTA | 3198 | OG1 | THR H | 204 | -8.377 | 9.169 | 39.197 | 1.00 69.69 | H | 0 |
| | ATOM | 3199 | CG2 | THR H | 204 | -7.367 | 11.021 | 40.346 | 1.00 68.98 | H | C |
| 30 | MOTA | 3200 | N | LYS H | | -9.444 | 13.779 | 38.899 | 1.00 71.84 | H | N |
| 30 | | | | | | | | | | | |
| | MOTA | 3201 | CA | LYS H | | -9.041 | 15.171 | 38.824 | 1.00 72.92 | H | C |
| | MOTA | 3202 | C | LYS H | 205 | -8.508 | 15.512 | 40.206 | 1.00 70.26 | H | C |
| | ATOM | 3203 | 0 | LYS H | | -9.036 | 15.027 | 41.200 | 1.00 70.61 | H | 0 |
| | | | | | | | | | | | |
| | MOTA | 3204 | CB | LYS H | | -10.240 | 16.055 | 38.479 | 1.00 76.81 | H | C |
| 35 | MOTA | 3205 | CG | LYS H | 205 | -9.928 | 17.541 | 38.480 | 1.00 93.84 | Ħ | C |
| | ATOM | 3206 | CD | LYS H | 205 | -11.159 | 18.374 | 38.140 | 1.00119.23 | H | C |
| | | 3207 | | | | -10.866 | 19.875 | 38.218 | 1.00127.13 | H | č |
| | ATOM | | CE | LYS H | | | | | | | |
| | MOTA | 3208 | NZ | LYS H | 205 | -10.500 | 20.334 | 39.593 | 1.00118.10 | H | N |
| | MOTA | 3209 | N | VAL H | 206 | -7.455 | 16.323 | 40.273 | 1.00 71.24 | H | N |
| 40 | ATOM | 3210 | CA | VAL H | | -6.865 | 16.710 | 41.554 | 1.00 65.47 | H | C |
| 40 | | | | | | | | | | | |
| | MOTA | 3211 | С | VAL H | | -6.097 | 18.015 | 41.458 | 1.00 66.88 | H | C |
| | ATOM | 3212 | 0 | VAL H | 206 | -5.419 | 18.270 | 40.464 | 1.00 63.59 | H | 0 |
| | MOTA | 3213 | CB | VAL H | 206 | -5.879 | 15.648 | 42.080 | 1.00 60.18 | H | C |
| | | | | | | | | 43.341 | | | Č |
| | ATOM | 3214 | | VAL H | | -5.211 | 16.151 | | 1.00 59.04 | H | |
| 45 | MOTA | 3215 | CG2 | VAL H | | -6.595 | 14.354 | 42.363 | 1.00 58.52 | H | C |
| | ATOM | 3216 | N | ASP H | 207 | -6.211 | 18.835 | 42.502 | 1.00 70.84 | H | N |
| | ATOM | 3217 | | ASP H | | -5.512 | 20.119 | 42.581 | 1.00 72.83 | H | Ċ |
| | | | | | | | | | | | |
| | ATOM | 3218 | С | ASP H | 207 | -4.636 | 20.118 | 43.832 | 1.00 72.60 | H | С |
| | ATOM | 3219 | 0 | ASP H | 207 | -5.119 | 19.821 | 44.927 | 1.00 75.84 | H | 0 |
| 50 | MOTA | 3220 | CB | ASP H | | -6.511 | 21.278 | 42.659 | 1.00 71.33 | H | C |
| -00 | | | | | | | | | | | |
| | ATOM | 3221 | CG | ASP H | | -7.287 | 21.477 | 41.364 | 1.00 77.68 | H | C |
| | MOTA | 3222 | OD1 | . ASP H | 207 | -6.681 | 21.899 | 40.354 | 1.00 80.92 | H | 0 |
| | MOTA | 3223 | 002 | ASP H | 207 | -8.508 | 21.207 | 41.352 | 1.00 90.49 | H | 0 |
| | | | | | | | | 43.672 | | | |
| | MOTA | 3224 | N | LYS H | | -3.353 | 20.439 | | 1.00 71.66 | H | N |
| 55 | ATOM | 3225 | CA | LYS H | 208 | -2.431 | 20.471 | 44.805 | 1.00 67.72 | H | C |
| | MOTA | 3226 | С | LYS H | 208 | -1.774 | 21.829 | 45.029 | 1.00 67.29 | H | C |
| | | | | | | | 22.387 | | | H | |
| | MOTA | 3227 | 0 | LYS H | | -1.123 | | 44.143 | 1.00 60.51 | | 0 |
| | ATOM | 3228 | CB | LYS H | 208 | -1.348 | 19.408 | 44.645 | 1.00 61.97 | H | C |
| | MOTA | 3229 | CG | LYS H | | -1.885 | 18.004 | 44.650 | 1.00 70.11 | H | C |
| 60 | | 3230 | | LYS H | | -2.596 | 17.706 | 45.952 | 1.00 79.56 | H | Č |
| OU. | MOTA | | CD | | | | | | | | |
| | MOTA | 3231 | CE | LYS H | | -1.633 | 17.728 | 47.136 | 1.00 79.20 | H | C |
| | MOTA | 3232 | NZ | LYS H | 208 | -2.313 | 17.296 | 48.397 | 1.00 74.65 | H | N |
| | MOTA | 3233 | N | LYS H | | -1.959 | 22.348 | 46.235 | 1.00 68.04 | H | N |
| | | | | | | | | | | | |
| | MOTA | 3234 | $^{\mathrm{CA}}$ | LYS H | | -1.396 | 23.624 | 46.632 | 1.00 68.05 | H | C |
| 65 | MOTA | 3235 | C | LYS H | 209 | -0.056 | 23.336 | 47.309 | 1.00 68.52 | H | C |
| | ATOM | 3236 | Ö | LYS H | | 0.067 | 22.404 | 48.111 | 1.00 68.41 | H | 0 |
| | | | | | | | | | | H | |
| | MOTA | 3237 | CB | LYS H | | -2.364 | 24.326 | 47.594 | 1.00 69.90 | | č |
| | MOTA | 3238 | CG | LYS H | | -1.838 | 25.586 | 48.257 | 1.00 66.76 | H | C |
| | ATOM | 3239 | CD | LYS H | | -2.792 | 26.024 | 49.348 | 1.00 78.35 | H | С |
| | | | | | | | | | | | _ |

| | ATOM MOTA | 3240 3241 | CE NZ | | 1 209 1 209 | -2.194 -3.031 | 27.115 27.382 | 50.220 51.432 | 1.00 94.10 1.00 96.38 | H H | C N |
|----|--------------|--------------|----------|-------|----------------|--------------------|-------------------|--------------------|--------------------------|--------|--------|
| | ATOM | 3242 | N | | 1 210 1 210 | 0.948 | 24.135 | 46.975 | 1.00 69.42 | H | N |
| 5 | ATOM ATOM | 3243 3244 | CA C | | 1 210 | 2.323 2.654 | 23.907 24.760 | 47.378 48.593 | 1.00 69.31 1.00 73.85 | H H | C |
| Ū | ATOM | 3245 | ŏ | ILE E | I 210 | 2.905 | 25.965 | 48.538 | 1.00 72.23 | H | ŏ |
| | MOTA | 3246 | CB | | I 210 | 3.289 | 24.189 | 46.204 | 1.00 63.42 | H | C |
| | ATOM ATOM | 3247 3248 | CG1 | ILE H | | 2.763 4.654 | 23.606 23.519 | 44.883 46.467 | 1.00 55.85 1.00 53.59 | H | C |
| 10 | ATOM | 3249 | | ILE I | | 2.724 | 22.077 | 44.880 | 1.00 33.39 | H H | C |
| | TER | 3250 | 022 | ILE I | f 210 | 21,21 | | | 2.00 12.00 | | Ŭ |
| | MOTA | 3251 | $s_{_}$ | SO4 | | -12.465 | 8.279 | -5.420 | 1.00139.70 | Z | ន |
| | MOTA | 3252 | 05 | SO4 | | -11.496 -13.354 | 7.532 | -4.640 | 1.00128.34 | Z | 0 |
| 15 | MOTA MOTA | 3253 3254 | 02 03 | SO4 2 | | -13.354 -11.721 | 9.016 8.960 | -4.584 -6.420 | 1.00133.20 1.00143.54 | Z Z | 0 |
| | MOTA | 3255 | 04 | SO4 | | -13.284 | 7.173 | -6.136 | 1.00137.69 | Z | ŏ |
| | TER | 3256 | | SO4 | | | | | | | |
| | MOTA ATOM | 3257 3258 | 0 | HOH I | | 6.642 28.229 | 26.255 27.688 | 11.504 14.335 | 1.00 44.22 1.00 47.65 | W | 0 |
| 20 | MOTA | 3259 | . 0 | HOH I | | 4.085 | 20.721 | 15.240 | 1.00 47.85 | W | 0 |
| | MOTA | 3260 | Ö | нон Т | | -2.722 | 25.529 | 5.319 | 1.00 43.81 | W | ŏ |
| | MOTA | 3261 | 0 | Т НОН | | -0.482 | 15.335 | 20.340 | 1.00 56.36 | W | 0 |
| | MOTA ATOM | 3262 3263 | 0 | HOH I | | -9.832 -1.203 | 15.976 25.888 | -2.164 -0.428 | 1.00 56.06 1.00 50.40 | W | 0 |
| 25 | MOTA | 3264 | 0 | HOH I | | -10.065 | 13.544 | 33.937 | 1.00 50.40 | W | 0 |
| | MOTA | 3265 | ŏ | HOH I | | -4.782 | 15.152 | -5.651 | 1.00 58.18 | W | ŏ |
| | MOTA | 3266 | 0 | нон г | | -3.602 | 22.705 | 2.193 | 1.00 48.13 | W | 0 |
| | ATOM ATOM | 3267 3268 | 0 | HOH I | | -11.748 12.028 | 12.731 16.121 | -2.744 18.701 | 1.00 46.32 1.00 41.71 | W | 0 |
| 30 | MOTA | 3269 | Ö | HOH I | | 3.379 | -3.325 | 0.685 | 1.00 44.58 | W | 0 |
| | MOTA | 3270 | Ō | HOH I | | 17.930 | 21.064 | 55.610 | 1.00 32.59 | . W | Ŏ |
| | ATOM | 3271 | 0 | HOH ! | | -0.999 | 21.444 | 1.050 | 1.00 39.37 | W | 0 |
| | ATOM ATOM | 3272 3273 | 0 | HOH I | | -7.188 11.612 | 20.691 6.022 | 15.900 14.835 | 1.00 58.62 1.00 63.80 | . W. | 0 |
| 35 | ATOM | 3273 | 0 | HOH I | | -21.984 | 9.843 | 5.129 | 1.00 63.80 | W W | 0 |
| | MOTA | 3275 | ŏ | нон у | | -13.113 | ~7.726 | 18.949 | 1.00 55.85 | W | ŏ |
| | MOTA | 3276 | 0 | HOH Y | | 11.899 | 30.835 | 17.167 | 1.00 51.40 | W | 0 |
| | ATOM ATOM | 3277 3278 | 0 | HOH I | | 5.068 10.249 | 4.550 11.292 | 7.254 38.205 | 1.00 66.68 1.00 65.97 | W | 0 |
| 40 | ATOM | 3279 | ŏ | HOH I | | 8.242 | 27.276 | 13.281 | 1.00 40.53 | M | ő |
| | MOTA | 3280 | Ō | HOH V | W 24 | 27.126 | 25.654 | 13.317 | 1.00 36.28 | W | Ö |
| | ATOM | 3281 | 0 | HOH I | | -2.011 | 21.099 | 11.221 | 1.00 36.94 | W | 0 |
| | ATOM ATOM | 3282 3283 | 0 | HOH I | | 4.152 3.465 | $14.440 \\ 8.412$ | $20.408 \\ 20.717$ | 1.00 44.38 1.00 36.27 | W | 0 |
| 45 | ATOM | 3284 | ŏ | HOH I | | -3.739 | 26.158 | -0.964 | 1.00 59.49 | W | ŏ |
| | ATOM | 3285 | 0 | HOH ! | | 8.758 | 15.447 | 18.540 | 1.00 58.26 | W | 0 |
| | ATOM | 3286 | 0 | HOH ! | | 11.634 | 3.618 | 7.590 | 1.00 64.90 | W | 0 |
| | ATOM ATOM | 3287 3288 | 0 | HOH I | | 9.169 21.365 | 11.593 7.678 | 35.533 8.159 | 1.00 53.91 1.00 56.30 | W. | 0 |
| 50 | ATOM | 3289 | ŏ | HOH 1 | | 1.667 | 26.705 | -2.342 | 1.00 34.36 | W | ŏ |
| | MOTA | 3290 | 0 | HOH 1 | | -0.777 | 2.920 | -5.893 | 1.00 54.04 | W | 0 |
| | MOTA MOTA | 3291 3292 | 0 | HOH I | | -1.979 6.580 | 6.414 2.378 | -4.690 7.003 | 1.00 86.59 1.00 56.10 | W | 0 |
| | MOTA | 3293 | Ö | HOH ! | | 8.782 | 3.265 | 5.256 | 1.00 35.26 | M | 0 |
| 55 | ATOM | 3294 | Ö | HOH | | 16.061 | 8.450 | 10.733 | 1.00 59.25 | W | ŏ |
| | MOTA | 3295 | 0 | HOH ! | | 29.645 | 4.189 | 52.482 | 1.00 54.67 | W | 0 |
| | MOTA MOTA | 3296 3297 | 0 | HOH Y | | 20.575 -22.962 | 4.765 11.039 | 61.334 19.094 | 1.00 68.62 1.00 73.88 | W | 0 |
| | ATOM | 3298 | 0 | HOH ' | | -21.174 | 11.687 | 21.368 | 1.00 73.88 | W | 0 |
| 60 | ATOM | 3299 | ō | HOH | | -18.934 | 22.014 | 5.912 | 1.00 60.22 | W | ŏ |
| | ATOM | 3300 | 0 | HOH | | 10.166 | 1.139 | 9.698 | 1.00 47.40 | M | 0 |
| | MOTA MOTA | 3301 3302 | 0 | HOH ' | | -16.050 16.088 | 3.113 23.610 | 11.263 39.697 | 1.00 37.96 1.00 46.51 | W | 0 |
| | ATOM | 3302 | 0 | HOH ! | | 2.897 | 30.138 | 2.027 | 1.00 48.31 | W | 0 |
| 65 | ATOM | 3304 | ŏ | HOH ' | w 48 | 24.057 | 1.224 | 45.686 | 1.00 48.96 | M | ŏ |
| | MOTA | 3305 | 0 | HOH ' | | 23.165 | 21.916 | 7.479 | 1.00 66.86 | W | 0 |
| | MOTA MOTA | 3306 3307 | 0 | HOH ' | | -11.702 -12.219 | 14.692 -0.922 | $23.074 \\ 1.076$ | 1.00 50.02 1.00 43.82 | M | 0 |
| | MOTA | 3308 | ŏ | HOH ' | | 12.391 | 12.245 | 37.897 | 1.00 49.94 | W | ő |
| | | | | | | | | | | | |

| | •- | | | | | | | | | | |
|----|------|------|---|-------|----|--------|--------|--------|------------|---|---|
| | ATOM | 3309 | 0 | HOH W | 53 | 4.767 | 11.266 | 29.449 | 1.00 43.95 | W | 0 |
| | MOTA | 3310 | 0 | HOH W | 54 | -3.099 | 21.164 | 48.329 | 1.00 58.57 | W | 0 |
| | MOTA | 3311 | 0 | HOH W | 55 | 12.781 | 10.766 | 29.425 | 1.00 53.41 | W | 0 |
| | ATOM | 3312 | 0 | HOH W | 56 | 14.923 | 28.548 | 3.207 | 1.00 58.18 | W | 0 |
| 5 | MOTA | 3313 | 0 | HOH W | 57 | 16.115 | 16.431 | -9.571 | 1.00 69.88 | W | 0 |
| | MOTA | 3314 | 0 | HOH W | 58 | 21.324 | 3.649 | 64.100 | 1.00 72.27 | W | 0 |
| | MOTA | 3315 | 0 | HOH W | 59 | 23.726 | 4.646 | 63.378 | 1.00 57.04 | W | 0 |
| | ATOM | 3316 | 0 | HOH W | 60 | 2.050 | 32.040 | 3.673 | 1.00 51.78 | W | 0 |
| | MOTA | 3317 | 0 | HOH W | 61 | 2.457 | 33.745 | 5.919 | 1.00 56.71 | W | 0 |
| 10 | MOTA | 3318 | 0 | HOH W | 62 | 8.951 | -2.545 | -6.773 | 1.00 54.15 | W | 0 |
| | MOTA | 3319 | 0 | HOH W | 63 | -6.141 | 27.599 | 9.560 | 1.00 51.61 | W | 0 |
| | ATOM | 3320 | 0 | HOH W | 64 | 10.484 | 22.284 | 28.826 | 1.00 50.78 | W | 0 |
| | TER | 3321 | | HOH W | 64 | | | | | | |

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^aAmino acids residues of the light (L) and heavy (H) chains are numbered according to the Chothia numbering system shown in Tables 6 and 7, respectively. ^bColumns are labeled according to Protein Data Bank Format, Version 2.2

Table 11. Structure coordinates of human IL-13/mAb13.2 Faba, b

| | Table II. | # # | Jamo | Por | Ch: | ain Res | # | X | <u>ин 111-1.</u> У | Z | occ | - В | SegID | Fla |
|-----|--------------|-----------------|------------------|------------|------|---------------|----|--------------|-----------------------|--------------------|------|----------------|-----------------|-------------|
| | | # 1 | vaille | RED. | C116 | alli ves | 11 | Λ | Ţ | Д | occ | ь | Segin | DTE |
| | ATOM | 1 | N | ASP | | 1 | | .935 | | 103.296 | | 32.51 | L | M |
| 5 | ATOM | 2 | CA | ASP | | 1 | | .850 | | 102.305 | | 31.66 | L | C |
| | ATOM | 3 | C | ASP | | 1 | | .682 | | 102.873 | | 33.17 | Ŀ | C |
| | ATOM ATOM | 4 5 | O CB | ASP ASP | | 1 1 | | .895 .401 | | 104.096 102.115 | | 35.13 32.59 | L L | 0 |
| | ATOM | 6 | CG | ASP | | 1 | | .478 | | 101.733 | | 38.56 | r L | Ğ |
| 10 | ATOM | 7 | | ASP | | 1 | | .953 | | 101.564 | | 32.48 | L | ŏ |
| | ATOM | 8 | | ASP | | 1 | | .273 | -5.483 | 101.616 | 1.00 | 40.42 | L | 0 |
| | MOTA | 9 | N | ILE | | 2 | | .224 | | 101.987 | 1.00 | 28.09 | L | N |
| | | 10 | CA | ILE | | 2 | | .045 | | 102.451 | | 25.55 | $ar{	extbf{r}}$ | C |
| 4.5 | | 11 | C | ILE ILE | | 2 | | .091 .173 | | 102.909 102.186 | | 24.79 23.23 | L L | C |
| 15 | | 12 13 | O CB | ILE | | 2 2 | | .965 | | 102.100 | | 24.03 | r L | C |
| | | $\frac{13}{14}$ | CG1 | | | 2 | | .822 | -2.608 | | | 23.16 | Ĺ | č |
| | | 15 | CG2 | ILE | | 2 | | .837 | -0.288 | 101.800 | | 21.56 | L | C |
| | ATOM : | 16 | CD1 | ILE | | 2 2 | | .903 | -2.205 | 99.809 | | 25.01 | L | С |
| 20 | | 17 | N | VAL | | 3 | | .345 | | 104.091 | | 19.63 | Ŀ | N |
| | | 18 | CA | VAL | | 3 | | .480 | 0.748 | | | 23.36 | Ŀ | C |
| | | 19 20 | C O | VAL VAL | | 3 3 | | .211 .377 | | 104.535 104.919 | | 20.65 17.60 | L L | C O |
| | | 21 | CB | VAL | | 3 | | .136 | | 106.139 | | 25.72 | Ľ | Ç |
| 25 | | 22 | | VAL | | 3 | | .351 | | 106.702 | | 18.81 | L | С |
| | | 23 | | VAL | | 3 | | .339 | -0.857 | | 1.00 | 24.17 | L | C |
| | | 24 | N | LEU | | 4 | | .508 | | 104.059 | | 14.42 | L | \tilde{N} |
| | | 25 | CA | LEU | | 4 | | .161 | | 103.883 | | 18.70 | L | C |
| 20 | | 26 27 | C O | LEU LEU | | $\frac{4}{4}$ | | .546 .327 | | 104.877 104.897 | | 18.25 17.11 | L L | 0 |
| 30 | | 28 | CB | LEU | | 4 | | .915 | | 102.460 | | 17.37 | L | Č |
| | | 29 | CG | LEU | | 4 | | .456 | 4.027 | | | 18.48 | L | Č |
| | | 30 | | LEU | | 4 | 21 | .321 | 4.756 | 99.972 | 1.00 | 21.81 | L | C |
| | | 31 | CD2 | LEU | | 4 | | .892 | | | | 10.40 | L | C |
| 35 | | 32 | N | THR | | 5 | | .397 | 5.948 | | | 17.41 | L | N |
| | | 33 | CA | THR | | 5 | | .896 | 6.865 8.274 | 106.687 106.385 | | 16.63 15.60 | L L | C C |
| | | 34 35 | C O | THR THR | | 5 5 | | .375 .582 | 8.522 | | | 18.70 | L | Õ |
| | | 36 | CB | THR | | 5 | | .394 | 6.433 | | | 20.60 | Ŀ | č |
| 40 | | 37 | | THR | | 5 | | .969 | 5.078 | | | 20.77 | L | Ō |
| | MOTA | 38 | CG2 | THR | L | 5 | | .809 | | | | 10.87 | L | C |
| | | 39 | N | GLN | | 6 | | .429 | 9.174 | | | 14.48 | L | N |
| | | 40 | CA | GLN | | 6 | | .786 | 10.551 11.432 | | | 19.27 20.35 | L L | C C |
| 45 | | 41 42 | C O | GLN GLN | | 6 6 | | .774 | 11.432 11.191 | | 1.00 | | L | Ö |
| 40 | | 43 | СВ | GLN | | 6 | | .848 | | 104.796 | | 15.21 | L | Č |
| | | $\frac{1}{4}$ | CG | GLN | | 6 | | .026 | | | 1.00 | 18.45 | L | C |
| | MOTA | 45 | $^{\mathtt{CD}}$ | GLN | | 6 | | .185 | | 102.327 | | 11.83 | L | С |
| | | 46 | | GLN | | 6 | | .438 | | 101.640 | | 18.94 | L | 0 |
| 50 | | 47 | | GLN | | 6 | | .304 .629 | | 102.179 107.115 | | 17.09 22.15 | L L | N |
| | | 48 49 | N CA | SER SER | | 7 7 | | .659 | | 108.226 | | 23.60 | L | C |
| | | 50 | C | SER | | 7 | | .105 | | 107.717 | | 22.73 | L | č |
| | | 51 | Ö | SER | | 7 | | .919 | | 106.800 | | 20.83 | L | 0 |
| 55 | MOTA | 52 | CB | SER | L | 7 | | .626 | | 109.313 | | 21.45 | L | C |
| | | 53 | OG | SER | | 7 | | .935 | | 108.812 | | 36.06 | L | 0 |
| | | 54 | N | PRO | | 8 | | .476 | | 108.238 | | 21.92 | L | N |
| | | 55 56 | CA C | PRO PRO | | 8 8 | | .388 | | 109.237 108.500 | | 17.23 18.60 | L L | C C |
| 60 | | 57 | Ö | PRO | | 8 | | .129 | | 107.288 | | 18.30 | L | ŏ |
| 00 | | 58 | СВ | PRO | | 8 | | .352 | | 109.770 | | 16.36 | Ľ | Č |
| | | 59 | CG | PRO | | 8 | 20 | .657 | 18.012 | 108.547 | 1.00 | 15.96 | L | C |
| | ATOM | 60 | CD | PRO | | 8 | | .871 | | 107.933 | | 16.22 | L | C |
| 0.7 | | 61 | N | ALA | | 9 | | .992 | | 109.217 | | 21.69 | L | N |
| 65 | | 62 63 | CA C | ALA ALA | | 9 9 | | .728 | | 108.575 107.883 | | 20.93 23.87 | L L | C C |
| | | 64 | 0 | ALA | | 9 | | .597 | | 106.847 | | 23.97 | L L | ŏ |
| | ATOM | 65 | СВ | ALA | | 9 | | .664 | | 109.609 | | 16.15 | Ľ | Č |
| | | | | | | | | | | | | | | |

| | | M GDD T 10 | 16.645 | 17.501 108.463 | 1.00 23.97 | L | N |
|----|--------------|--------------------------------------|------------------|----------------------------------|--------------------------|--------------------|--------|
| | ATOM ATOM | 66 N SER L 10 67 CA SER L 10 | | 18.779 107.890 | 1.00 23.55 | ŗ | Ĉ |
| | MOTA | 68 C SER L 10 | 17.394 | 19.757 108.162 | 1.00 20.78 | L | C |
| | ATOM | 69 O SER L 10 | | 19.669 109.245 | 1.00 20.28 | $	ilde{	extbf{r}}$ | 0 |
| 5 | MOTA | 70 CB SER L 10 | | 19.288 108.657 | 1.00 19.45 1.00 36.04 | L L | C |
| | MOTA | 71 OG SER L 10 | | 20.370 107.960 20.652 107.203 | 1.00 36.04 1.00 16.86 | L | И |
| | ATOM | 72 N LEU L 11 73 CA LEU L 11 | | 21.642 107.298 | 1.00 10.36 | Ľ | Ç |
| | ATOM ATOM | 73 CA LEU L 11 74 C LEU L 11 | | 22.969 106.760 | 1.00 17.41 | Ŀ | Ĉ |
| 10 | ATOM ATOM | 75 O LEU L 11 | 17.601 | 22.996 105.724 | 1.00 20.59 | L | 0 |
| 10 | ATOM | 76 CB LEU L 11 | | 21.175 106.395 | 1.00 21.77 | L | C |
| | ATOM | 77 CG LEU L 11 | | 22.165 106.165 | 1.00 24.51 | L | C |
| | ATOM | 78 CD1 LEU L 11 | | 22.491 107.531 | 1.00 36.89 | Ŀ | C |
| | MOTA | 79 CD2 LEU L 11 | | 21.573 105.281 | 1.00 37.85 | L | C N |
| 15 | ATOM | 80 N ALA L 12 | | 24.079 107.460 | 1.00 16.76 1.00 17.17 | L L | C |
| | ATOM | 81 CA ALA L 12 | | 25.373 106.956 26.247 106.827 | 1.00 17.17 | L | Č |
| | MOTA | 82 C ALA L 12 83 O ALA L 12 | | 26.279 107.755 | 1.00 10.24 | Ŀ | Ö |
| | MOTA MOTA | 83 O ALA L 12 84 CB ALA L 12 | | 26.062 107.931 | 1,00 12.64 | L | Č |
| 20 | ATOM | 85 N VAL L 13 | | 26.909 105.698 | 1.00 13.87 | L | N |
| 20 | MOTA | 86 CA VAL L 13 | | 27.848 105.538 | 1.00 13.69 | L | C |
| | ATOM | 87 C VAL L 13 | | 29.106 104.907 | 1.00 17.25 | Ŀ | C |
| | MOTA | 88 O VAL L 13 | | 29.117 104.336 | 1.00 21.72 | L | 0 |
| | MOTA | 89 CB VAL L 13 | | 27.286 104.656 | 1.00 15.08 1.00 10.62 | L L | C |
| 25 | MOTA | 90 CG1 VAL L 13 | | 25.958 105.301 27.096 103.157 | 1.00 10.62 1.00 9.18 | L L | C |
| | ATOM | 91 CG2 VAL L 13 92 N SER L 14 | | 30.202 105.000 | 1.00 15.71 | L | N |
| | MOTA MOTA | 92 N SER L 14 93 CA SER L 14 | | 31.440 104.326 | 1.00 14.91 | L | C |
| | ATOM | 94 C SER L 14 | 20.796 | 31.365 102.849 | 1.00 14.49 | L | С |
| 30 | ATOM | 95 O SER L 14 | 21.709 | 30.635 102.423 | 1.00 13.93 | L | 0 |
| • | MOTA | 96 CB SER L 14 | 21.203 | 32.682 104.941 | 1.00 11.69 | Ē | C |
| | MOTA | 97 OG SER L 14 | 20.999 | 32.727 106.352 | 1.00 18.48 | L | 0 |
| | ATOM | 98 N LEU L 15 | 20.079 | 32.137 102.048 | 1.00 13.89 1.00 16.79 | L L | C N |
| | MOTA | 99 CA LEU L 15 | 20.330 21.824 | 32.173 100.620 32.522 100.384 | 1.00 16.79 1.00 17.38 | Ľ | Č |
| 35 | MOTA | 100 C LEU L 15 | 22.354 | 33.409 101.025 | 1.00 21.74 | L | ō |
| | ATOM ATOM | 101 O LEU L 15 102 CB LEU L 15 | 19.462 | 33.258 99.927 | 1.00 14.69 | L | С |
| | MOTA | 102 CG LEU L 15 | 17.926 | 32.958 99.764 | 1.00 34.86 | L | С |
| | MOTA | 104 CD1 LEU L 15 | 17.184 | 34.159 99.090 | 1.00 44.91 | L | C |
| 40 | ATOM | 105 CD2 LEU L 15 | | 31.665 98.905 | 1.00 32.56 | <u>r</u> | C |
| | ATOM | 106 N GLY L 16 | | 31.805 99.483 | 1.00 16.14 | L | C N |
| | MOTA | 107 CA GLY L 16 | | 32.089 99.144 31.323 99.964 | 1.00 12.82 1.00 14.60 | L L | c |
| | MOTA | 108 C GLY L 16 | | 31.323 99.964 31.335 99.602 | 1.00 14.00 | L | õ |
| 45 | ATOM | 109 O GLY L 10 110 N GLN L 13 | | 30.683 101.063 | 1.00 10.34 | L | N |
| 45 | MOTA MOTA | 111 CA GLN L 1 | | 29.914 101.882 | 1.00 12.15 | L | C |
| | MOTA | 112 C GLN L 1 | | 28.502 101.325 | 1.00 13.53 | L | С |
| | ATOM | 113 O GLN L 1 | 24.873 | 28.108 100.371 | 1.00 14.77 | L | 0 |
| | ATOM | 114 CB GLN L 1 | | 29.775 103.318 | 1.00 17.40 | L | G G |
| 50 | MOTA | 115 CG GLN L 1 | | 31.111 104.106 | 1.00 10.18 1.00 17.90 | L L | C |
| | ATOM | 116 CD GLN L 1 | | 30.902 105.540 30.187 105.905 | 1.00 17.90 | L | Ö |
| | MOTA | 117 OE1 GLN L 1' 118 NE2 GLN L 1' | | 31.478 106.386 | 1.00 4.74 | Ľ | Ŋ |
| | MOTA MOTA | 118 NE2 GLN L 1' 119 N ARG L 1 | | 27.763 101.953 | 1.00 13.19 | L | N |
| 55 | ATOM | 120 CA ARG L 1 | | 26.389 101.515 | 1.00 15.63 | L | C |
| 00 | ATOM | 121 C ARG L 1 | | 25.437 102.374 | 1.00 15.34 | Ŀ | C |
| | ATOM | 122 O ARG L 1 | | 25.619 103.595 | 1.00 19.40 | L | 0 |
| | ATOM | 123 CB ARG L 1 | | 26.066 101.682 | 1.00 15.02 | L | C |
| | MOTA | 124 CG ARG L 1 | | 24.566 101.572 | 1.00 25.18 1.00 39.56 | L L | C |
| 60 | MOTA | 125 CD ARG L 1 | | 24.166 102.211 24.654 101.453 | 1.00 39.56 | L | И |
| | ATOM | 126 NE ARG L 1 | | 25.885 101.533 | 1.00 04.48 | L | Ç |
| | ATOM | 127 CZ ARG L 1 128 NH1 ARG L 1 | | 26.777 102.353 | 1.00 86.83 | L | Ŋ |
| | MOTA MOTA | 128 NH1 ARG L 1 129 NH2 ARG L 1 | | 26.225 100.788 | 1.00 82.59 | L | N |
| 65 | MOTA | 130 N ALA L 1 | | 24.396 101.752 | 1.00 17.11 | L | N |
| | ATOM | 131 CA ALA L 1 | 24.505 | 23.379 102.489 | 1.00 12.89 | Ŀ | C |
| | MOTA | 132 C ALA L 1 | 25.198 | 22.031 102.204 | 1.00 16.54 | L | C |
| | MOTA | 133 O ALA L 1 | | 21.713 101.026 | 1.00 22.79 | L | 0 |
| | ATOM | 134 CB ALA L 1 | 23.054 | 23.294 101.953 | 1.00 14.85 | L | C |

| | | | ·m· - | **** | | | | | | |
|----|-----------------|-----|-------------|----------------------------|----|--------|----------------|------------|---------|---|
| | ATOM | 135 | N | THR L | 20 | 25.476 | 21.265 103.249 | 1.00 14.17 | L | N |
| | ATOM | 136 | | THR L | 20 | 26.096 | 19.960 103.054 | 1.00 15.56 | L | Ĉ |
| | | | | | | | 18.934 103.752 | 1.00 15.65 | | |
| | ATOM | 137 | | THR L | 20 | 25.227 | | | Ŀ | C |
| | ATOM | 138 | 0 | THR L | 20 | 24.813 | 19.126 104.923 | 1.00 20.89 | Ŀ | 0 |
| 5 | MOTA | 139 | CB | THR L | 20 | 27.533 | 19.985 103.630 | 1.00 17.90 | L | C |
| | MOTA | 140 | OG1 | THR L | 20 | 28.291 | 20.901 102.832 | 1.00 23.27 | L | 0 |
| | MOTA | 141 | CG2 | THR L | 20 | 28.202 | 18.608 103.594 | 1.00 20.09 | L | С |
| | ATOM | 142 | N | ILE L | 21 | 24.896 | 17.877 103.035 | 1.00 14.46 | L | N |
| | ATOM | 143 | CA | ILE L | 21 | 24.066 | 16.841 103.610 | 1.00 18.34 | L | Ĉ |
| 40 | | | | | | | 15.504 103.500 | 1.00 10.54 | L | |
| 10 | ATOM | 144 | C | ILE L | 21 | 24.760 | | | | С |
| | ATOM | 145 | 0 | ILE L | 21 | 25.495 | 15.251 102.542 | 1.00 18.26 | L | 0 |
| | MOTA | 146 | CB | ILE L | 21 | 22.648 | 16.809 103.010 | 1.00 19.09 | L | C |
| | MOTA | 147 | CG1 | ILE L | 21 | 22.648 | 16.401 101.575 | 1.00 29.56 | L | C |
| | MOTA | 148 | CG2 | ILE L | 21 | 21.985 | 18.173 103.154 | 1.00 23.73 | L | С |
| 15 | ATOM | 149 | CD1 | ILE L | 21 | 21.219 | 16.545 100.967 | 1.00 37.88 | L | С |
| ,0 | ATOM | 150 | N | SER L | 22 | 24.559 | 14.651 104.492 | 1.00 15.94 | L | N |
| | | | CA | SER L | 22 | 25.286 | 13.391 104.429 | 1.00 20.98 | L | Ĉ |
| | ATOM | 151 | | | | | | | L | Č |
| | MOTA | 152 | C | SER L | 22 | 24.467 | 12.148 104.321 | 1.00 18.51 | | |
| | MOTA | 153 | 0 | SER L | 22 | 23.269 | 12.123 104.622 | 1.00 20.37 | L | 0 |
| 20 | \mathbf{MOTA} | 154 | CB | SER L | 22 | 26.244 | 13.290 105.598 | 1.00 17.26 | L | С |
| | MOTA | 155 | OG | SER L | 22 | 25.516 | 13.126 106.775 | 1.00 38.04 | ${f L}$ | 0 |
| | ATOM | 156 | N | CYS L | 23 | 25.107 | 11.099 103.822 | 1.00 15.15 | L | N |
| | MOTA | 157 | CA | CYS L | 23 | 24.383 | 9.833 103.656 | 1.00 19.93 | L | C |
| | ATOM | 158 | C | CYS L | 23 | 25.370 | 8.749 104.099 | 1.00 19.09 | L | C |
| 25 | MOTA | 159 | ŏ | CYS L | 23 | 26.497 | 8.706 103.609 | 1.00 24.06 | Ē | ŏ |
| 25 | | | | | | 24.047 | 9.641 102.175 | 1.00 18.33 | L | č |
| | ATOM | 160 | CB | CYS L | 23 | | - | | L | |
| | MOTA | 161 | SG | CYS L | 23 | 23.310 | 8.045 101.699 | 1.00 19.01 | | S |
| | MOTA | 162 | N | LYS L | 24 | 24.961 | 7.869 105.013 | 1.00 19.81 | L | N |
| | ATOM | 163 | $^{\rm CA}$ | LYS L | 24 | 25.876 | 6.835 105.490 | 1.00 21.44 | L | C |
| 30 | ATOM | 164 | C | LYS L | 24 | 25.312 | 5.482 105.148 | 1.00 19.45 | ${f L}$ | C |
| | MOTA | 165 | 0 | LYS L | 24 | 24.168 | 5.216 105.416 | 1.00 17.29 | L | 0 |
| | MOTA | 166 | CB | LYS L | 24 | 26.089 | 6.960 107.018 | 1.00 20.14 | L | С |
| | ATOM | 167 | CG | LYS L | 24 | 26.987 | 5.848 107.576 | 1.00 38.35 | L | С |
| | ATOM | 168 | CD | LYS L | 24 | 27.320 | 6.037 109.086 | 1.00 55.69 | L | Ċ |
| 35 | ATOM | 169 | CE | LYS L | 24 | 28.358 | 7.158 109.343 | 1.00 65.78 | L | č |
| 33 | | | | | 24 | 27.749 | 8.535 109.135 | 1.00 73.97 | Ĺ | N |
| | MOTA | 170 | NZ | LYS L | | | | | | |
| | ATOM | 171 | N | ALA L | 25 | 26.122 | 4.613 104.564 | 1.00 16.58 | Ŀ | И |
| | MOTA | 172 | CA | ALA L | 25 | 25.595 | 3.290 104.192 | 1.00 20.95 | L | C |
| | MOTA | 173 | С | ALA L | 25 | 26.021 | 2.214 105.224 | 1.00 20.06 | L | С |
| 40 | ATOM | 174 | 0 | ALA L | 25 | 27.130 | 2.293 105.753 | 1.00 21.66 | L | 0 |
| | MOTA | 175 | CB | $\mathtt{ALA}\ \mathtt{L}$ | 25 | 26.141 | 2.885 102.822 | 1.00 16.44 | ${f L}$ | C |
| | MOTA | 176 | N | SER L | 26 | 25.176 | 1.214 105.434 | 1.00 20.89 | ${f L}$ | N |
| | MOTA | 177 | CA | SER L | 26 | 25.502 | 0.134 106.403 | 1.00 24.53 | L | С |
| | ATOM | 178 | C | SER L | 26 | 26.614 | -0.805 105.917 | 1.00 24.48 | L | С |
| 45 | MOTA | 179 | ō | SER L | 26 | 27.258 | -1.521 106.720 | 1.00 25.97 | L | 0 |
| .0 | MOTA | 180 | ČВ | SER L | 26 | 24.234 | -0.680 106.758 | 1.00 20.85 | L | C |
| | ATOM | 181 | OG | SER L | 26 | 23.577 | -1.189 105.615 | 1.00 24.47 | _ L | õ |
| | | 182 | | | 27 | 26.848 | -0.797 104.598 | 1.00 25.23 | L | N |
| | MOTA | | N | GLU L | | | -1.606 103.971 | 1.00 22.24 | Ŀ | Č |
| | ATOM | 183 | CA | GLU L | 27 | 27.889 | | | | |
| 50 | MOTA | 184 | C | GLU L | 27 | 28.484 | -0.723 102.886 | 1.00 22.04 | Ŀ | C |
| | ATOM | 185 | 0 | GLU L | 27 | 27.831 | 0.237 102.428 | 1.00 25.83 | Ŀ | 0 |
| | MOTA | 186 | CB | GLU L | 27 | 27.293 | -2.881 103.288 | 1.00 16.57 | L | C |
| | MOTA | 187 | CG | GLU L | 27 | 26.251 | -3.624 104.048 | 1.00 17.06 | L | С |
| | MOTA | 188 | CD | GLU L | 27 | 25.816 | -4.858 103.275 | 1.00 25.63 | L | С |
| 55 | ATOM | 189 | OE1 | GLU L | 27 | 24.831 | -5.516 103.672 | 1.00 18.33 | 占 | 0 |
| | MOTA | 190 | OE2 | GLU L | 27 | 26.515 | -5.132 102.264 | 1.00 23.85 | L | 0 |
| | MOTA | 191 | N | SER L | 28 | 29.698 | -1.029 102.455 | 1.00 23.92 | Ŀ | N |
| | ATOM | 192 | ČA | SER L | 28 | 30.355 | -0.237 101.412 | 1.00 20.04 | L | Ĉ |
| | | | | | 28 | 29.562 | -0.293 100.128 | 1.00 21.07 | L | č |
| 00 | MOTA | 193 | C | SER L | | | | | | |
| 60 | ATOM | 194 | 0 | SER L | | 28.967 | -1.329 99.782 | 1.00 23.98 | L | 0 |
| | MOTA | 195 | CB | SER L | 28 | 31.779 | -0.778 101.121 | 1.00 18.95 | L | C |
| | ATOM | 196 | OG | SER L | 28 | 32.408 | -0.078 100.037 | 1.00 28.13 | ŗ | 0 |
| | MOTA | 197 | N | VAL L | 29 | 29.570 | 0.798 99.383 | 1.00 18.22 | Ŀ | N |
| | MOTA | 198 | $^{\rm CA}$ | VAL L | 29 | 28.829 | 0.788 98.103 | 1.00 17.79 | L | С |
| 65 | MOTA | 199 | C | VAL L | 29 | 29.840 | 0.937 96.981 | 1.00 19.59 | L | C |
| | ATOM | 200 | 0 | VAL L | 29 | 29.465 | 1.207 95.837 | 1.00 22.01 | L | 0 |
| | MOTA | 201 | СВ | VAL L | 29 | 27.766 | 1.940 98.010 | 1.00 17.51 | L | С |
| | MOTA | 202 | | VAL L | 29 | 26.675 | 1.740 99.072 | 1.00 12.98 | L | C |
| | ATOM | 203 | | VAL L | 29 | 28.441 | 3.326 98.172 | 1.00 16.63 | L | Č |
| | 224 024 | | 202 | | | | | | | - |

| | | 001 | | | | | 0 700 | | 4 00 17 00 | | _ | |
|-----|--------------|------------|------------------|----------------|------------|------------------|------------------|------------------|--------------------------|---|----|--------|
| | MOTA | 204 | N | ASP L | 30 | 31.127 | 0.708 | 97.279 | 1.00 17.33 | | | N |
| | MOTA | 205 | CA | ASP L | 30 | 32.178 | 0.849 | 96.268 | 1.00 18.23 | | | C |
| | MOTA | 206 | C | ASP L | 30 | 32.339 | -0.453 | 95.497 | 1.00 19.53 | - | | C |
| _ | ATOM | 207 | 0 | ASP L | 30 | 32.219 | -1.559 | 96.071 | 1.00 26.39 | | | 0 |
| 5 | ATOM | 208 | CB | ASP L | 30 | 33.534 | 1.153 | 96.908 | 1.00 12.12 | | | C |
| | ATOM | 209 | CG | ASP L | 30 | 33.662 | 2.592 | 97.326 | 1.00 22.31 | | | C |
| | MOTA | 210 | | ASP L | 30 | 34.761 | 2.975 | 97.764 | 1.00 29.89 | | | 0 |
| | MOTA | 211 | | ASP L | 30 | 32.676 | 3.331 | 97.208 | 1.00 18.13 | | | 0 |
| | MOTA | 212 | N | ASN L | 30A | 32.617 | -0.316 | 94.206 | 1.00 20.90 | | | N |
| 10 | ATOM | 213 | CA | ASN L | 30A | 32.797 | -1.499 | 93.344 | 1.00 22.44 | | | C |
| | ATOM | 214 | C | ASN L | 30A | 34.090 | -1.203 | 92.623 | 1.00 23.21 | | | C |
| | ATOM | 215 | 0 | ASN L | 30A | 34.141 | -0.339 | 91.735 | 1.00 25.31 | | | 0 |
| | MOTA | 216 | CB | ASN L ASN L | 30A | 31.693 | -1.594 | 92.283 | 1.00 20.72 | | | C |
| 4.5 | MOTA | 217 218 | CG | | 30A 30A | 31.884 | -2.785 -3.934 | 91.384 91.852 | 1.00 24.84 1.00 24.37 | | | С О |
| 15 | MOTA MOTA | 219 | ND2 | ASN L ASN L | 30A | 31.800 32.149 | -3.934 -2.530 | 90.071 | 1.00 24.37 | | | И |
| | | 220 | | | 30B | 35.161 | -2.330 -1.861 | 93.051 | 1.00 23.26 | | | N |
| | MOTA | 221 | N | TYR L | 30B | 36.460 | -1.651 | 92.445 | 1.00 23.88 | | | C |
| | ATOM ATOM | 222 | CA C | TYR L TYR L | 30B | 36.823 | -0.230 | 92.173 | 1.00 21.04 | | | Č |
| 20 | ATOM | 223 | 0 | TYR L | 30B | 37.123 | 0.166 | 91.038 | 1.00 21.35 | | | õ |
| 20 | MOTA | 224 | CB | TYR L | 30B | 36.567 | -2.494 | 91.176 | 1.00 21.55 | | | Č |
| | ATOM | 225 | CG | TYR L | 30B | 36.520 | -3.965 | 91.534 | 1.00 26.67 | | L | C |
| | ATOM | 226 | CD1 | | 30B | 37.580 | -4.556 | 92.215 | 1.00 17.83 | | | Č |
| | ATOM | 227 | CD2 | TYR L | 30B | 35.427 | -4.754 | 91.211 | 1.00 30.04 | | | č |
| 25 | ATOM | 228 | CE1 | | 30B | 37.542 | -5.890 | 92.556 | 1.00 28.99 | | L | Č |
| | ATOM | 229 | CE2 | TYR L | 30B | 35.375 | -6.104 | 91.553 | 1.00 38.10 | | | Č |
| | MOTA | 230 | CZ | TYR L | 30B | 36.445 | -6.657 | 92.229 | 1.00 32.14 | | Li | C |
| | MOTA | 231 | OH | TYR L | 30B | 36.429 | -7.974 | 92.591 | 1.00 34.61 | | | 0 |
| | MOTA | 232 | N | GLY L | 30C | 36.774 | 0.560 | 93.236 | 1.00 20.14 | | L | N |
| 30 | MOTA | 233 | CA | GLY L | 30C | 37.178 | 1.951 | 93.126 | 1.00 21.20 | : | L | C |
| | MOTA | 234 | С | GLY L | 30C | 36.101 | 2.933 | 92.676 | 1.00 25.36 | | | C |
| | MOTA | 235 | 0 | GLY L | 30C | 36.355 | 4.122 | 92.635 | 1.00 29.51 | | | 0 |
| | MOTA | 236 | N | LYS L | 30D | 34.925 | 2.437 | 92.306 | 1.00 22.83 | | | N |
| | MOTA | 237 | $^{\mathrm{CA}}$ | LYS L | 30D | 33.833 | 3.328 | 91.845 | 1.00 23.04 | | | С |
| 35 | ATOM | 238 | С | LYS L | 30D | 32.767 | 3.306 | 92.943 | 1.00 22.36 | | | C |
| | ATOM | 239 | 0 | LYS L | 30D | 32.407 | 2.230 | 93.382 | 1.00 17.33 | | | 0 |
| | ATOM | 240 | CB | LYS L | 30D | 33.195 | 2.807 | 90.554 | 1.00 24.66 | | | C |
| | ATOM | 241 | CG | LYS L | 30D | 33.949 | 3.156 | 89.277 | 1.00 29.64 | | | C |
| 40 | ATOM | 242 243 | CD | LYS L LYS L | 30D 30D | 35.097 34.641 | 2.195 0.783 | 88.997 88.732 | 1.00 26.58 1.00 21.88 | | | C C |
| 40 | ATOM ATOM | 243 | CE NZ | LYS L | 30D | 35.869 | -0.054 | 88.518 | 1.00 21.33 | | | N |
| | ATOM | 245 | N | SER L | 31 | 32.263 | 4.488 | 93.362 | 1.00 16.41 | | | N |
| | ATOM | 246 | CA | SER L | 31 | 31.266 | 4.493 | 94.450 | 1.00 14.47 | | | C |
| | ATOM | 247 | C | SER L | 31 | 29.876 | 4.552 | 93.817 | 1.00 12.87 | | | Č |
| 45 | ATOM | 248 | Ö | SER L | 31 | 29.559 | 5.508 | 93.135 | 1.00 17.73 | | | ō |
| | ATOM | 249 | CB | SER L | 31 | 31.528 | 5.718 | 95.369 | 1.00 13.31 | | | C |
| | MOTA | 250 | OG | SER L | 31 | 32.772 | 5.543 | 96.018 | 1.00 9.74 | | L | 0 |
| | MOTA | 251 | \mathbf{N} | LEU L | 32 | 29.068 | 3.533 | 94.047 | 1.00 14.84 | : | L | N |
| | MOTA | 252 | CA | LEU L | 32 | 27.737 | 3.444 | 93.414 | 1.00 15.21 | | | С |
| 50 | MOTA | 253 | С | LEU L | 32 | 26.661 | 4.109 | 94.271 | 1.00 15.33 | | | С |
| | ATOM | 254 | 0 | LEU L | 32 | 25.759 | 3.444 | 94.743 | 1.00 15.90 | | | 0 |
| | ATOM | 255 | CB | LEU L | 32 | 27.410 | 1.946 | 93.122 | 1.00 14.19 | | L | C |
| | ATOM | 256 | CG | LEU L | 32 | 28.528 | 1.268 | 92.240 | 1.00 16.68 | | | C |
| EE | MOTA | 257 | | LEU L | 32 | 28.098 | -0.113 | 91.812 | 1.00 19.02 | | | C |
| 55 | MOTA | 258 | | LEU L | 32 | 28.841 | 2.115 | 90.956 | 1.00 16.75 | | | C |
| | ATOM ATOM | 259 260 | N CA | MET L MET L | 33 33 | 26.805 25.858 | 5.422 6.243 | 94.446 95.228 | 1.00 15.14 1.00 15.51 | | | C |
| | ATOM | 261 | CA | MET L | 33 | 25.424 | 7.400 | 94.306 | 1.00 13.31 | | | C |
| | ATOM | 262 | o | MET L | 33 | 26.268 | 8.060 | 93.664 | 1.00 14.69 | | | Ö |
| 60 | MOTA | 263 | CB | MET L | 33 | 26.522 | 6.857 | 96.482 | 1.00 16.89 | | | Č |
| 00 | ATOM | 264 | CG | MET L | 33 | 25.438 | 7.575 | 97.437 | 1.00 11.58 | | | č |
| | ATOM | 265 | SD | MET L | 33 | 24.457 | 6.317 | 98.203 | 1.00 25.28 | | | Š |
| | ATOM | 266 | CE | MET L | 33 | 25.482 | 5.831 | 99.589 | 1.00 11.25 | | | č |
| | ATOM | 267 | N | HIS L | 34 | 24.114 | 7.621 | 94.239 | 1.00 11.24 | | | Ŋ |
| 65 | ATOM | 268 | CA | HIS L | 34 | 23.566 | 8.649 | 93.369 | 1.00 10.81 | | | С |
| | ATOM | 269 | C | HIS L | 34 | 22.672 | 9.529 | 94.235 | 1.00 13.28 | | | С |
| | ATOM | 270 | 0 | HIS L | 34 | 22.163 | 9.062 | 95.283 | 1.00 7.46 | | | 0 |
| | ATOM | 271 | CB | HIS L | 34 | 22.709 | 7.988 | 92.278 | 1.00 9.21 | | | C |
| | ATOM | 272 | CG | HIS L | 34 | 23.392 | 6.816 | 91.619 | 1.00 19.51 | | L | С |

| | | | | | **** ****** | | | | | | |
|----|------|-----|-------------|------------------------|-------------|--------|--------|---------|------------|--------|----------|
| | ATOM | 273 | ND1 | HIS L | 34 | 24.568 | 6.950 | 90.896 | 1.00 18.89 | I | . NT |
| | ATOM | 274 | | HIS L | 34 | 23.061 | 5.501 | 91.562 | | | |
| | | 275 | | HIS L | | | | | 1.00 19.95 | I | |
| | ATOM | | | | 34 | 24.932 | 5.770 | 90.429 | 1.00 8.56 | I | - |
| _ | MOTA | 276 | | HIS L | 34 | 24.037 | 4.874 | 90.815 | 1.00 18.35 | I | \sim N |
| 5 | MOTA | 277 | N | TRP L | 35 | 22.478 | 10.770 | 93.806 | 1.00 11.97 | I | ı N |
| | MOTA | 278 | ca | TRP L | 35 | 21.658 | 11.731 | 94.603 | 1.00 14.22 | I | |
| | ATOM | 279 | C | TRP L | 35 | 20.557 | 12.321 | 93.730 | 1.00 14.57 | Ī | |
| | ATOM | 280 | ŏ | TRP L | 35 | | | | | | |
| | | | | | | 20.793 | 12.665 | 92.577 | 1.00 13.68 | I | _ |
| | ATOM | 281 | CB | TRP L | 35 | 22.525 | 12.914 | 95.123 | 1.00 12.34 | I | , C |
| 10 | ATOM | 282 | CG | TRP L | 35 | 23.529 | 12.532 | 96.148 | 1.00 18.11 | I | G C |
| | ATOM | 283 | CD1 | TRP L | 35 | 24.842 | 12.167 | 95.941 | 1.00 13.80 | I | |
| | ATOM | 284 | CD2 | | 35 | 23.346 | 12.610 | 97.560 | 1.00 15.53 | | |
| | | | | | | | | | | Ī | |
| | ATOM | 285 | NE1 | | 35 | 25.491 | 12.027 | 97.158 | 1.00 7.32 | I | |
| | ATOM | 286 | CE2 | TRP L | 35 | 24.588 | 12.302 | 98.164 | 1.00 10.41 | I | , C |
| 15 | MOTA | 287 | CE3 | TRP L | 35 | 22.242 | 12.928 | 98.381 | 1.00 22.77 | I | |
| | ATOM | 288 | CZ2 | TRP L | 35 | 24.756 | 12.300 | 99.551 | 1.00 16.39 | I | |
| | ATOM | 289 | CZ3 | | 35 | 22.396 | 12.933 | 99.730 | 1.00 10.74 | | |
| | | | | | | | | | | I | |
| | ATOM | 290 | CH2 | | 35 | 23.643 | 12.622 | 100.320 | 1.00 11.41 | I | - |
| | ATOM | 291 | N | TYR L | 36 | 19.362 | 12.470 | 94.306 | 1.00 13.73 | I | ı N |
| 20 | ATOM | 292 | ca | TYR L | 36 | 18.212 | 13.005 | 93.593 | 1.00 13.32 | I | , C |
| | ATOM | 293 | C | TYR L | 36 | 17.614 | 14.178 | 94.360 | 1.00 12.87 | I | |
| | ATOM | 294 | Ó | TYR L | 36 | 17.681 | 14.233 | 95.579 | 1.00 11.74 | Ī | |
| | ATOM | 295 | СВ | TYR L | | 17.081 | | | | | |
| | | | | | 36 | | 11.942 | 93.464 | 1.00 13.04 | I | |
| | ATOM | 296 | CG | TYR L | 36 | 17.545 | 10.667 | 92.771 | 1.00 11.47 | I | |
| 25 | ATOM | 297 | CD1 | TYR L | 36 | 18.207 | 9.660 | 93.488 | 1.00 9.50 | I | , C |
| | ATOM | 298 | CD2 | TYR L | 36 | 17.398 | 10.526 | 91.391 | 1.00 12.45 | E | |
| | ATOM | 299 | CE1 | | 36 | 18.739 | 8.534 | 92.820 | 1.00 12.96 | I | |
| | | 300 | | | | | | | | | |
| | ATOM | | CE2 | | 36 | 17.907 | 9.414 | 90.729 | 1.00 10.42 | L | |
| | ATOM | 301 | CZ | TYR L | 36 | 18.578 | 8.436 | 91.445 | 1.00 12.56 | L | , C |
| 30 | MOTA | 302 | OH | TYR L | 36 | 19.180 | 7.385 | 90.768 | 1.00 13.38 | L | . 0 |
| | ATOM | 303 | N | GLN L | 37 | 16.981 | 15.072 | 93.620 | 1.00 10.25 | I | |
| | ATOM | 304 | CA | GLN L | 37 | 16.254 | 16.180 | 94.252 | 1.00 11.70 | Ī | |
| | | | | | | | | | | | |
| | ATOM | 305 | C | GLN L | 37 | 14.783 | 15.956 | 93.941 | 1.00 13.16 | L | |
| | MOTA | 306 | 0 | GLN L | 37 | 14.444 | 15.606 | 92.794 | 1.00 17.26 | L | , 0 |
| 35 | MOTA | 307 | CB | GLN L | 37 | 16.649 | 17.515 | 93.600 | 1.00 10.59 | L | C |
| | ATOM | 308 | CG | GLN L | 37 | 15.845 | 18.749 | 94.028 | 1.00 10.72 | I | |
| | MOTA | 309 | CD | GLN L | 37 | 16.206 | 19.926 | 93.103 | 1.00 15.26 | | |
| | | | | | | | | | | L | |
| | MOTA | 310 | OE1 | | 37 | 15.916 | 19.885 | 91.887 | 1.00 16.02 | L | . 0 |
| | ATOM | 311 | NE2 | GLN L | 37 | 16.857 | 20.947 | 93.659 | 1.00 13.48 | L | N |
| 40 | ATOM | 312 | N | GLN L | 38 | 13.916 | 16.212 | 94.921 | 1.00 17.77 | L | N |
| | ATOM | 313 | CA | GLN L | 38 | 12.470 | 16.140 | 94.680 | 1.00 20.77 | L | |
| | ATOM | 314 | C | GLN L | 38 | 11.804 | 17.343 | 95.326 | 1.00 21.40 | | |
| | | | | - | | | | | | L | |
| | ATOM | 315 | 0 | GLN L | 38 | 11.828 | 17.509 | 96.563 | 1.00 22.63 | L | _ |
| | MOTA | 316 | CB | GLN L | 38 | 11.835 | 14.901 | 95.313 | 1.00 19.42 | L | , C |
| 45 | MOTA | 317 | CG | GLN L | 38 | 10.354 | 14.805 | 94.968 | 1.00 13.86 | L | ı C |
| | MOTA | 318 | CD | GLN L | 38 | 9.748 | 13.498 | 95.491 | 1.00 19.68 | L | |
| | MOTA | 319 | OE1 | | 38 | 10.122 | 13.011 | 96.545 | 1.00 14.26 | L | |
| | | | | | | | | | | - | _ |
| | ATOM | 320 | | GLN L | 38 | 8.834 | 12.935 | 94.726 | 1.00 19.99 | L | |
| | MOTA | 321 | N | LYS L | 39 | 11.254 | 18.170 | 94.457 | 1.00 24.73 | L | N |
| 50 | MOTA | 322 | CA | LYS L | 39 | 10.505 | 19.355 | 94.879 | 1.00 26.95 | Ŀ | C |
| | ATOM | 323 | C | LYS L | 39 | 9.047 | 18.965 | 95.083 | 1.00 31.28 | L | |
| | ATOM | 324 | Ō | LYS L | 39 | 8.492 | 18.004 | 94.493 | 1.00 27.67 | | |
| | | | | | | | | | | L | |
| | ATOM | 325 | CB | LYS L | 39 | 10.624 | 20.467 | 93.817 | 1.00 25.37 | L | |
| | ATOM | 326 | CG | LYS L | 39 | 12.024 | 20.994 | 93.607 | 1.00 28.24 | L | |
| 55 | ATOM | 327 | $^{\rm CD}$ | LYS L | 39 | 12.109 | 21.962 | 92.440 | 1.00 25.89 | L | C |
| | ATOM | 328 | CE | LYS L | 39 | 13.525 | 22.460 | 92.197 | 1.00 41.55 | _ L | |
| | ATOM | 329 | NZ | LYS L | 39 | 13.723 | 23.040 | 90.805 | | | |
| | | | | | | | | 90.005 | 1.00 39.62 | Ŀ | |
| | ATOM | 330 | N | PRO L | 40 | 8.384 | 19.708 | 95.969 | 1.00 37.71 | L | |
| | MOTA | 331 | ca | PRO L | 40 | 6.984 | 19.511 | 96.310 | 1.00 40.24 | L | |
| 60 | MOTA | 332 | C | PRO L | 40 | 6.129 | 19.315 | 95.045 | 1.00 37.39 | L | |
| | MOTA | 333 | 0 | PRO L | 40 | 6.226 | 20.104 | 94.122 | 1.00 35.53 | P _ | |
| | ATOM | 334 | СВ | PRO L | 40 | | | 97.036 | | | |
| | | | | | | 6.637 | 20.819 | | 1.00 44.21 | ŗ | |
| | ATOM | 335 | CG | PRO L | 40 | 7.926 | 21.168 | 97.729 | 1.00 42.86 | r | |
| | MOTA | 336 | CD | PRO L | 40 | 8.954 | 20.888 | 96.653 | 1.00 39.12 | L | C |
| 65 | MOTA | 337 | N | GLY L | 41 | 5.363 | 18.230 | 95.002 | 1.00 36.74 | L | |
| | ATOM | 338 | CA | GLY L | 41 | 4.506 | 17.946 | 93.862 | 1.00 36.85 | L | |
| | ATOM | 339 | C | GLY L | 41 | 5.202 | 17.572 | 92.568 | 1.00 35.88 | L | |
| | | | | | | | | | | | |
| | ATOM | 340 | 0 | GLY L | 41 | 4.576 | 17.503 | 91.523 | 1.00 35.09 | L | |
| | ATOM | 341 | N | GLN L | 42 | 6.510 | 17.325 | 92.626 | 1.00 35.27 | L | N |
| | | | | | | | | | | | |

| | MOTA MOTA | 342 343 | CA GLN L | 42 42 | 7.237 7.856 | | | 1.00 28.24 1.00 25.86 | | r c |
|----|--------------|----------------|------------------------|----------|------------------|------------------|------------------|--------------------------|--------|------------|
| | ATOM ATOM | 344 345 | O GLN L | 42 42 | 7.921 | 15.047 | 92.697 | 1.00 25.25 | | r o |
| 5 | ATOM | | CG GLN L | 42 42 | 8.386 7.950 | | 91.124 90.729 | 1.00 29.72 1.00 34.63 | | . c |
| | ATOM | | CD GLN L | 42 | 9.127 | 20.234 | 90.242 | 1.00 45.60 | | ت . 2 م |
| | MOTA ATOM | | OE1 GLN L NE2 GLN L | 42 42 | 8.965 | 21.421 | 90.002 | 1.00 50.47 | | 5 6 |
| | MOTA | | N SER L | 43 | 10.303 8.340 | 19.639 15.026 | 90.094 90.506 | 1.00 47.27 1.00 22.44 | | <u>N</u> |
| 10 | ATOM | 351 | CA SER L | 43 | 8.985 | 13.744 | 90.587 | 1.00 22.44 | | C N |
| | MOTA MOTA | | C SER L | 43 | 10.490 | 13.988 | 90.930 | 1.00 21.02 | Ī | _ |
| | ATOM | | O SER L CB SER L | 43 43 | 10.986 8.831 | 15.104 13.041 | 90.802 | 1.00 19.00 | I | 0 |
| | MOTA | | OG SER L | 43 | 9.851 | 13.443 | 89.213 88.334 | 1.00 24.31 1.00 31.71 | I | - |
| 15 | ATOM | | N PRO L | 44 | 11.186 | 12.953 | 91.401 | 1.00 19.03 | I | _ |
| | MOTA ATOM | | CA PRO L C PRO L | 44 44 | 12.619 13.403 | 13.056 | 91.738 | 1.00 19.57 | I | ı C |
| | MOTA | | O PRO L | 44 | 12.971 | 13.344 12.997 | 90.454 89.339 | 1.00 19.17 1.00 17.27 | I | _ |
| 00 | ATOM | | CB PRO L | 44 | 12.963 | 11.675 | 92.304 | 1.00 20.33 | I | _ |
| 20 | MOTA MOTA | | CG PRO L | 44 44 | 11.568 | 11.163 | 92.901 | 1.00 14.26 | I | C |
| | ATOM | | N ALA L | 45 | 10.630 14.576 | 11.645 13.942 | 91.786 90.603 | 1.00 17.98 1.00 14.94 | I | _ |
| | MOTA | 364 | CA ALA L | 45 | 15.400 | 14.217 | 89.428 | 1.00 14.94 | I I | |
| 25 | ATOM | | C ALA L | 45 | 16.833 | 13.921 | 89.846 | 1.00 15.71 | Ī | |
| 20 | MOTA MOTA | | O ALA L | 45 45 | 17.287 15.300 | 14.318 | 90.927 | 1.00 14.34 | I | 0 |
| | MOTA | | N LEU L | 46 | 17.545 | 15.702 13.285 | 89.000 88.948 | 1.00 17.79 1.00 15.14 | Ţ | _ |
| | ATOM | | CA LEU L | 46 | 18.948 | 12.903 | 89.212 | 1.00 11.85 | I. | |
| 30 | MOTA MOTA | | C LEU L O LEU L | 46 46 | 19.841 | 14.154 | 89.206 | 1.00 12.85 | L | C |
| 00 | ATOM | | CB LEU L | 46 | 19.825 19.416 | 14.944 11.894 | 88.247 88.107 | 1.00 12.83 1.00 9.18 | L | |
| | MOTA | 373 (| CG LEU L | 46 | 20.875 | 11.408 | 88.320 | 1.00 9.18 1.00 8.52 | L L | _ |
| | ATOM | | CD1 LEU L | 46 | 21.074 | 10.591 | 89.660 | 1.00 8.06 | L | |
| 35 | ATOM ATOM | | CD2 LEU L N LEU L | 46 47 | 21.269 | 10.533 | 87.111 | 1.00 7.61 | L | C |
| | MOTA | | CA LEU L | 47 | 20.630 21.578 | 14.323 15.439 | 90.277 90.384 | 1.00 11.81 1.00 11.37 | Ŀ | |
| | ATOM | | C LEU L | 47 | 23.038 | 15.014 | 90.150 | 1.00 11.37 | L L | - |
| | ATOM ATOM | | O LEU L | 47 | 23.774 | 15.649 | 89.393 | 1.00 13.32 | L | 0 |
| 40 | ATOM | | CG LEU L | 47 47 | 21.556 20.215 | 15.997 16.587 | 91.789 92.289 | 1.00 11.40 1.00 11.75 | L | _ |
| | MOTA | 382 (| CD1 LEU L | 47 | 20.362 | 16.812 | 93.810 | 1.00 11.75 | L L | _ |
| | ATOM ATOM | | CD2 LEU L | 47 | 19.911 | 17.879 | 91.522 | 1.00 4.80 | L | č |
| | ATOM | | N ILE L CA ILE L | 48 48 | 23.422 24.800 | 13.952 13.468 | 90.856 | 1.00 12.53 | L | N |
| 45 | MOTA | 386 (| C ILE L | 48 | 24.821 | 11.953 | 90.883 90.754 | 1.00 10.52 1.00 14.33 | L L | C |
| | ATOM | | O ILE L | 48 | 24.066 | 11.263 | 91.443 | 1.00 16.13 | L | Ö |
| | MOTA MOTA | | CB ILE L CG1 ILE L | 48 | 25.444 | 13.826 | 92.281 | 1.00 11.93 | · L | Ċ |
| | ATOM | | CG2 ILE L | 48 48 | 25.465 26.842 | 15.351 13.136 | 92.495 92.431 | 1.00 9.28 1.00 11.58 | L | C |
| 50 | MOTA | 391 C | CD1 ILE L | 48 | 26.422 | 16.165 | 91.519 | 1.00 14.29 | L L | C C |
| | ATOM ATOM | 392 N 393 C | | 49 | 25.651 | 11.424 | 89.860 | 1.00 12.80 | L | Ŋ |
| | ATOM | 394 C | | 49 49 | 25.698 27.118 | 9.977 9.484 | 89.790 90.107 | 1.00 14.45 | L | C |
| | MOTA | 395 C | O TYR L | 49 | 28.114 | 10.177 | 89.869 | 1.00 13.75 1.00 14.87 | L L | C |
| 55 | ATOM | | CB TYR L | 49 | 25.223 | 9.449 | 88.419 | 1.00 6.50 | Ľ | č |
| | ATOM ATOM | | CG TYR L | 49 49 | 26.079 27.100 | 9.899 | 87.246 | 1.00 14.44 | L | С |
| | ATOM | | D2 TYR L | 49 | 25.840 | 9.105 11.131 | 86.733 86.646 | 1.00 9.63 1.00 20.17 | L | C |
| 00 | MOTA | 400 C | CE1 TYR L | 49 | 27.876 | 9.531 | 85.632 | 1.00 20.17 | L L | C |
| 60 | ATOM ATOM | | CE2 TYR L | 49 | 26.620 | 11.584 | 85.542 | 1.00 22.28 | L | С |
| | ATOM | | CZ TYR L OH TYR L | 49 49 | 27.624 28.372 | 10.778 11.257 | 85.049 | 1.00 20.57 | L | C |
| | MOTA | 404 N | | 50 | 27.176 | 8.279 | 83.987 90.648 | 1.00 19.11 1.00 14.11 | L L | O |
| 65 | ATOM | | A ARG L | 50 | 28.461 | 7.617 | 90.962 | 1.00 16.52 | r r | N C |
| 65 | MOTA ATOM | 406 C 407 O | | 50 50 | 29.311 | 8.530 | 91.871 | 1.00 16.04 | L | C |
| | ATOM | | B ARG L | 50 | 30.480 29.228 | 8.795 7.293 | 91.583 89.673 | 1.00 14.95 1.00 12.62 | Ŀ | 0 |
| | MOTA | 409 C | G ARG L | 50 | 30.084 | 5.998 | 89.784 | 1.00 12.62 | L L | C |
| | ATOM | 410 C | D ARG L | 50 | 30.933 | 5.820 | 88.460 | 1.00 11.26 | Ĺ | Č |
| | | | | | | | | | | |

| | 7. (TIOM | // 1 | NE ADC I | 50 | 30.073 | 5.942 | 87.252 | 1.00 23.52 | L | N |
|-----|--------------|-------------------|------------------|------|------------------|------------------|------------------|--------------------------|---------|--------------------------|
| | ATOM ATOM | $\frac{411}{412}$ | NE ARG L | | 30.543 | 6.227 | 86.037 | 1.00 20.37 | L | C |
| | ATOM | 413 | NH1 ARG L | | 31.852 | 6.404 | 85.858 | 1.00 26.18 | L | N |
| | ATOM | 414 | NH2 ARG L | | 29.727 | 6.354 | 85.003 | 1.00 18.24 | L | N |
| 5 | MOTA | 415 | N ALA L | | 28.621 | 9.031 | 92.901 | 1.00 14.01 | L | N |
| | MOTA | 416 | CA ALA L | | 29.125 | 9.886 | 93.975 | 1.00 14.19 | Ŀ | C |
| | ATOM | 417 | C ALA L | | 29.531 | 11.309 | 93.680 | 1.00 16.63 | L | C |
| | ATOM | 418 | O ALA I | | 29.255 | 12.190 | 94.481 94.727 | 1.00 15.01 1.00 6.77 | L L | O C |
| 10 | MOTA MOTA | 419 420 | CB ALA L N SER L | | 30.288 30.119 | 9.177 11.555 | 92.509 | 1.00 14.35 | L | N |
| 10 | ATOM | 421 | CA SER L | | 30.652 | 12.887 | 92.214 | 1.00 12.90 | L | Ç |
| | ATOM | 422 | C SER L | | 30.437 | 13.427 | 90.815 | 1.00 10.83 | L | Č |
| | ATOM | 423 | O SER I | | 30.884 | 14.542 | 90.504 | 1.00 9.89 | L | 0 |
| | MOTA | 424 | CB SER L | | 32.179 | 12.851 | 92.476 | 1.00 5.64 | L | С |
| 15 | ATOM | 425 | OG SER L | | 32.747 | 11.797 | 91.672 | 1.00 19.18 | L | 0 |
| | ATOM | 426 | N ASN I | | 29.747 | 12.677 | 89.962 | 1.00 10.80 | L | N |
| | ATOM | 427 | CA ASN I | | . 29.575 | 13.143 | 88.561 | 1.00 6.02 1.00 13.29 | L L | G G |
| | MOTA | 428 | C ASN I | | 28.301 27.228 | 13.953 13.468 | 88.439 88.813 | 1.00 15.29 | L | Ö |
| 20 | ATOM ATOM | 429 430 | O ASN I | | 29.461 | 11.954 | 87.630 | 1.00 9.04 | L | č |
| 20 | MOTA | 431 | CG ASN I | | 30.756 | 11.172 | 87.594 | 1.00 15.97 | L | Č |
| | ATOM | 432 | OD1 ASN I | | 31.787 | 11.705 | 87.178 | 1.00 24.43 | L | 0 |
| | MOTA | 433 | ND2 ASN I | 53 | 30.730 | 9.948 | 88.079 | 1.00 23.89 | L | N |
| | MOTA | 434 | N LEU I | | 28.443 | 15.143 | 87.880 | 1.00 12.27 | L | $\widetilde{\mathbf{N}}$ |
| 25 | MOTA | 435 | CA LEU I | | 27.296 | 16.075 | 87.725 | 1.00 11.19 | Ţ | C |
| | ATOM | 436 | C LEU I | | 26.438 26.928 | 15.659 15.572 | 86.539 85.400 | 1.00 13.26 1.00 17.40 | L L | C |
| | MOTA MOTA | 437 438 | O LEU I | | 27.866 | 17.498 | 87.499 | 1.00 17.40 | L | č |
| | ATOM | 439 | CG LEU I | | 26.793 | 18.590 | 87.336 | 1.00 9.35 | L | č |
| 30 | ATOM | 440 | CD1 LEU I | | 26.013 | 18.667 | 88.688 | 1.00 11.24 | L | C |
| - • | MOTA | 441 | CD2 LEU I | 54 | 27.473 | 20.001 | 86.935 | 1.00 10.06 | L | C |
| | MOTA | 442 | N GLU I | | 25.152 | 15.437 | 86.792 | 1.00 13.19 | L | N |
| | ATOM | 443 | CA GLU I | | 24.271 | 15.056 | 85.715 | 1.00 13.50 | Ŀ | C |
| | ATOM | 444 | C GLU I | | 24.099 | 16.206 | 84.684 | 1.00 16.40 1.00 16.66 | L L | C |
| 35 | ATOM | 445 | O GLU I | | 23.952 22.935 | 17.356 14.633 | 85.035 86.323 | 1.00 17.40 | r r | Ċ |
| | ATOM ATOM | 446 447 | CB GLU I | | 21.891 | 14.257 | 85.238 | 1.00 17.40 | L | č |
| | MOTA | 448 | CD GLU I | | 22.174 | 12.930 | 84.538 | 1.00 21.37 | L | Č |
| | MOTA | 449 | OE1 GLU I | | 23.189 | 12.227 | 84.879 | 1.00 29.09 | Ŀ | 0 |
| 40 | ATOM | 450 | OE2 GLU I | | 21.366 | 12.583 | 83.642 | 1.00 14.35 | Ŀ | 0 |
| | MOTA | 451 | N SER I | | 24.141 | 15.873 | 83.390 | 1.00 18.45 | Ŀ | N |
| | MOTA | 452 | CA SER I | | 23.959 | 16.910 | 82.370 | 1.00 21.02 | L | C |
| | MOTA | 453 | C SER I | | 22.660 21.610 | 17.692 17.089 | 82.628 82.907 | 1.00 20.45 1.00 23.00 | L L | C |
| 45 | ATOM ATOM | 454 455 | O SER I | | 23.893 | 16.260 | 80.972 | 1.00 23.30 | L | č |
| -10 | ATOM | 456 | OG SER I | | 23.696 | 17.280 | 79.990 | 1.00 35.05 | L | ŏ |
| | ATOM | 457 | N GLY | | 22.735 | 19.017 | 82.564 | 1.00 16.05 | L | N |
| | ATOM | 458 | CA GLY I | 57 | 21.540 | 19.832 | 82.794 | 1.00 15.79 | L | C |
| | MOTA | 459 | C GLY I | | 21.383 | 20.336 | 84.219 | 1.00 17.48 | Ŀ | C |
| 50 | ATOM | 460 | O GLY I | | 20.604 | 21.239 | 84.470 | 1.00 20.76 | L | O |
| | ATOM | 461 | N ILE I | | 22.130 | 19.758 20.199 | 85.154 86.559 | 1.00 15.63 1.00 13.54 | L L | C N |
| | MOTA MOTA | 462 463 | CA ILE I | | 22.077 23.210 | 21.225 | 86.775 | 1.00 13.54 | L | č |
| | ATOM | 464 | O ILE | | 24.353 | 20.972 | 86.376 | 1.00 15.41 | L | ŏ |
| 55 | ATOM | 465 | CB ILE | | 22.321 | 18.985 | 87.479 | 1.00 16.14 | L | C |
| | MOTA | 466 | CG1 ILE I | | 21.248 | 17.925 | 87.205 | 1.00 10.84 | L | C |
| | MOTA | 467 | CG2 ILE I | | 22.293 | 19.433 | 88.957 | 1.00 14.42 | L | C |
| | ATOM | 468 | CD1 ILE I | | 19.771 | 18.436 | 87.373 | 1.00 7.96 | Ŀ | C |
| | MOTA | 469 | N PRO | | 22.933 | 22.351 | 87.471 | 1.00 16.57 | L | N |
| 60 | MOTA | 470 | CA PRO I | | 24.011 | 23.324 | 87.650 | 1.00 15.02 1.00 17.68 | L L | G G |
| | ATOM | 471 472 | C PRO 1 | | 25.127 24.888 | 22.857 22.119 | 88.586 89.551 | 1.00 17.88 | r r | 0 |
| | MOTA MOTA | 473 | O PRO I | | 23.296 | 24.567 | 88.181 | 1.00 20.01 | L | č |
| | ATOM | 474 | CG PRO | | 22.119 | 24.013 | 88.932 | 1.00 14.55 | Ĺ | č |
| 65 | ATOM | 475 | CD PRO | | 21.702 | 22.766 | 88.166 | 1.00 16.37 | L | С |
| | MOTA | 476 | N ALA | ւ 60 | 26.342 | 23.352 | 88.335 | 1.00 15.03 | Ľ | Ŋ |
| | MOTA | 477 | CA ALA | | 27.482 | 22.936 | 89.141 | 1.00 15.80 | L | C |
| | ATOM | 478 | C ALA | | 27.443 | 23.436 | 90.588 | 1.00 16.37 | L, L | O C |
| | ATOM | 479 | O ALA | L 60 | 28.370 | 23.164 | 91.349 | 1.00 14.10 | т | J |

| | ATOM | 480 | CB | ALA L | 60 | 28.828 | 23.389 | 9 88.439 | 1.00 19.03 | L | ~ |
|-------|--------------|------------|-----------|----------------|----------|------------------|------------------|--------------------|--------------------------|--------------------------|--------|
| | ATOM | 481 | N | ARG L | | 26.382 | | | 1.00 13.86 | L L | C N |
| | ATOM | 482 | CA | ARG L | | 26.259 | 24.48 | 5 92.408 | 1.00 12.66 | L | Č |
| 5 | ATOM ATOM | 483 484 | C O | ARG L | | 26.076 | | | 1.00 13.33 | \mathbf{r} | Č |
| 3 | ATOM | 485 | CB | ARG L | | 26.222 | 23.166 | | 1.00 11.62 | L | 0 |
| | MOTA | 486 | CG | ARG L | 61 | 25.015 24.958 | 25.355 26.567 | | 1.00 10.50 | Ŀ | C |
| | ATOM | 487 | CD | ARG L | | 23.759 | 27.528 | | 1.00 21.56 1.00 34.92 | L L | C |
| | MOTA | 488 | NE | ARG L | 61 | 22.428 | 27.036 | | 1.00 20.51 | L | C N |
| 10 | MOTA | 489 | CZ | ARG L | 61 | 21.594 | 26.438 | | 1.00 19.50 | Ľ | C |
| | ATOM | 490 | | L ARG L | 61 | 21.952 | 26.279 | | 1.00 20.76 | $\widetilde{\mathbf{L}}$ | Ŋ |
| | ATOM | 491 492 | | 2 ARG L | 61 | 20.455 | 25.955 | | 1.00 18.94 | L | N |
| | ATOM ATOM | 492 | N CA | PHE L | 62 | 25.682 | 22.086 | | 1.00 11.06 | L | N |
| 15 | ATOM | 494 | CA | PHE L | 62 62 | 25.545 26.816 | 20.771 19.968 | | 1.00 13.46 | L | C |
| | ATOM | 495 | ŏ | PHE L | 62 | 27.282 | 19.875 | | 1.00 14.58 | L | C |
| | ATOM | 496 | ĊВ | PHE L | 62 | 24.378 | 19.988 | | 1.00 14.64 1.00 10.25 | L L | 0 |
| | MOTA | 497 | CG | PHE L | 62 | 23.019 | 20.612 | | 1.00 10.23 | L L | C C |
| | ATOM | 498 | | PHE L | 62 | 22.359 | 20.344 | | 1.00 14.57 | L L | C |
| 20 | ATOM | 499 | | PHE L | 62 | 22.478 | 21.533 | 91.929 | 1.00 11.67 | $\widetilde{\mathbf{L}}$ | č |
| | MOTA | 500 | | PHE L | 62 | 21.175 | 20.994 | | 1.00 9.15 | L | Č |
| | ATOM ATOM | 501 502 | CE2 CZ | PHE L | 62 | 21.248 | 22.220 | | 1.00 5.02 | L | С |
| | ATOM | 503 | N | SER L | 62 63 | 20.631 27.354 | 21.932 | | 1.00 15.51 | L | C |
| 25 | MOTA | 504 | CA | SER L | 63 | 28.542 | 19.375 18.518 | | 1.00 13.28 | ŗ | И |
| | MOTA | 505 | C | SER L | 63 | 28.450 | 17.384 | 94.817 | 1.00 16.69 1.00 16.93 | L L | C |
| | MOTA | 506 | 0 | SER L | 63 | 27.740 | 17.512 | | 1.00 13.99 | . L | 0 C |
| | MOTA | 507 | CB | SER L | 63 | 29.841 | 19.326 | | 1.00 20.80 | . L | Č |
| 20 | ATOM | 508 | OG | SER L | 63 | 29.864 | 19.821 | 95.383 | 1.00 15.22 | ī | ŏ |
| 30 | MOTA MOTA | 509 | N | GLY L | 64 | 29.176 | 16.290 | | 1.00 15.15 | L | N |
| | MOTA | 510 511 | CA C | GLY L | 64 64 | 29.112 | 15.214 | | 1.00 12.85 | L | C |
| | ATOM | 512 | Ö | GLY L | 64 64 | 30.474 31.363 | 14.689 | | 1.00 17.05 | L | C |
| | MOTA | 513 | N | SER L | 65 | 30.657 | 14.813 14.097 | | 1.00 20.04 | L | 0 |
| 35 | ATOM | 514 | CA | SER L | 65 | 31.927 | 13.486 | | 1.00 14.74 1.00 17.90 | L L | N |
| | MOTA | 515 | C | SER L | 65 | 31.709 | 12.310 | | 1.00 17.90 | r r | C |
| | ATOM | 516 | 0 | SER L | 65 | 30.597 | 12.056 | | 1.00 10.29 | L | 0 |
| | ATOM | 517 | CB | SER L | 65 | 32.914 | 14.491 | 98.011 | 1.00 17.37 | L | č |
| 40 | ATOM ATOM | 518 | OG | SER L | 65 | 32.304 | 14.967 | 99.193 | 1.00 31.08 | Ŀ | 0 |
| 40 | ATOM | 519 520 | N CA | GLY L | 66 66 | 32.795 | 11.582 | 98.630 | 1.00 17.49 | L | N |
| | ATOM | 521 | C | GLY L | 66 | 32.711 33.145 | 10.462 9.168 | 99.551 98.886 | 1.00 12.08 | L | C |
| | MOTA | 522 | ŏ | GLY L | 66 | 33.445 | 9.144 | 97.696 | 1.00 17.57 1.00 20.81 | F | C |
| | ATOM | 523 | N | SER L | 67 | 33.215 | 8.099 | 99.673 | 1.00 20.81 | L L | O N |
| 45 | MOTA | 524 | CA | SER L | 67 | 33.591 | 6.784 | 99.170 | 1.00 17.33 | L | C |
| | ATOM | 525 | C | SER L | 67 | 33.241 | | 100.287 | 1.00 18.00 | L | č |
| | MOTA MOTA | 526 527 | 0 | SER L | 67 | 32.990 | | 101.444 | 1.00 16.60 | L | 0 |
| | ATOM | 528 | CB OG | SER L SER L | 67 67 | 35.103 | 6.694 | 98.886 | 1.00 14.43 | L | C |
| 50 | ATOM | 529 | И | ARG L | 68 | 35.792 33.193 | 6.817 4.550 | | 1.00 15.13 | $ar{\mathbf{L}}$ | 0 |
| | ATOM | 530 | CA | ARG L | 68 | 32.875 | | 99.906 100.793 | 1.00 18.02 1.00 21.90 | L | N |
| | MOTA | 531 | C | ARG L | 68 | 31.494 | 3.545 | 101.440 | 1.00 21.90 | L L | C |
| | ATOM | 532 | 0 | ARG L | 68 | 30.486 | 3.175 | 100.813 | 1.00 22.85 | L | C O |
| p= p= | ATOM | 533 | CB | ARG L | 68 | 34.003 | 3.352 | 101.843 | 1.00 22.76 | Ŀ | Č |
| 55 | ATOM | 534 | CG | ARG L | 68 | 35.389 | | 101.227 | 1.00 26.60 | L | č |
| | ATOM ATOM | 535 536 | CD | ARG L | 68 | 36.416 | | 102.374 | 1.00 48.13 | L | С |
| | ATOM | 537 | NE CZ | ARG L ARG L | 68 68 | 37.790 | 3.179 | 101.986 | 1.00 67.04 | L | N |
| | ATOM | 538 | | ARG L | 68 68 | 38.466 37.902 | 4.289 | 102.301 103.019 | 1.00 77.72 | L | C |
| 60 | ATOM | 539 | NH2 | ARG L | 68 | 39.737 | | 103.019 | 1.00 74.08 | L | N |
| | MOTA | 540 | N | THR L | 69 | 31.431 | | 102.691 | 1.00 83.92 1.00 24.77 | L | N |
| | ATOM | 541 | CA | THR L | 69 | 30.144 | | 103.374 | 1.00 24.77 | L L | C N |
| | MOTA | 542 | C | THR L | 69 | 29.698 | 5.545 | 103.712 | 1.00 26.51 | L | C |
| 85 | ATOM | 543 | 0 | THR L | 69 | 28.592 | 5.726 | 104.182 | 1.00 28.14 | L | ŏ |
| 65 | ATOM ATOM | 544 545 | CB OC1 | THR L | 69 | 30.158 | 3.306 | 104.710 | 1.00 26.91 | L | Č |
| | ATOM | 545 546 | | THR L | 69 69 | 31.166 | 3.856 | 105.554 | 1.00 27.96 | L | 0 |
| | ATOM | 547 | N | ASP L | 70 | 30.523 30.517 | | 104.424 103.434 | 1.00 25.31 | , L | C |
| | ATOM | 548 | CA | ASP L | 70 | 30.158 | | 103.434 | 1.00 20.56 1.00 22.63 | L | N |
| | | | | | | - 3,230 | ,,,,,,, | 200.000 | 1.00 44.03 | Þ | C |

| | ~ | E40 | C ASP L | 70 | 30.238 | 8 863 · | 102.615 | 1.00 20.68 | L | С |
|----|--------------|------------|------------------------|----------|------------------|------------------|--------------------|--------------------------|--------|--------|
| | ATOM ATOM | 549 550 | C ASP L O ASP L | 70 | 31.290 | 9.031 | 102.016 | 1.00 26.56 | L | õ |
| | ATOM | 551 | CB ASP L | 70 | 31.118 | 8.435 | 104.889 | 1.00 26.74 | L | С |
| | ATOM | 552 | CG ASP L | 70 | 31.033 | | 106.173 | 1.00 33.17 | L | C |
| 5 | ATOM | 553 | OD1 ASP L | 70 | 30.028 | | 106.878 106.428 | 1.00 45.62 1.00 48.35 | L L | 0 |
| | ATOM | 554 | OD2 ASP L N PHE L | 70 71 | 31.954 29.124 | | 100.428 | 1.00 48.33 | Ľ L | N |
| | ATOM ATOM | 555 556 | CA PHE L | 71 | 29.041 | | 101.185 | 1.00 18.07 | L | Ĉ |
| | MOTA | 557 | C PHE L | 71 | 28.411 | | 101.605 | 1.00 16.31 | L | C |
| 10 | ATOM | 558 | O PHE L | 71 | 27.691 | 11.797 | | 1.00 14.04 | L | 0 |
| | ATOM | 559 | CB PHE L | 71 | 28.138 | - | 100.109 | 1.00 16.27 | L | C |
| | ATOM | 560 | CG PHE L | 71 | 28.709 | 8.463 | 99.614 | 1.00 15.39 | L L | C |
| | MOTA | 561 | CD1 PHE L CD2 PHE L | 71 71 | 28.523 29.579 | 7.284 8.462 | 100.325 98.525 | 1.00 11.66 1.00 7.25 | L | C |
| 15 | ATOM ATOM | 562 563 | CE1 PHE L | 71 | 29.223 | 6.062 | 99.951 | 1.00 12.24 | L | č |
| 13 | ATOM | 564 | CE2 PHE L | 71 | 30.268 | 7.301 | 98.153 | 1.00 7.98 | L | C |
| | MOTA | 565 | CZ PHE L | 71 | 30.084 | 6.092 | 98.878 | 1.00 8.50 | L | C |
| | ATOM | 566 | N THR L | 72 | 28.624 | | 100.801 | 1.00 17.20 | Ŀ | Й |
| | ATOM | 567 | CA THR L | 72 | 27.998 | | 101.081 | 1.00 17.62 | L L | C C |
| 20 | MOTA | 568 | C THR L O THR L | 72 72 | 27.575 28.196 | 14.675 14.435 | 99.751 98.717 | 1.00 19.31 1.00 20.88 | L L | Ö |
| | ATOM ATOM | 569 570 | O THR L CB THR L | 72 | 28.964 | | 101.770 | 1.00 15.55 | L | č |
| | ATOM | 571 | OG1 THR L | 72 | 30.058 | | 100.913 | 1.00 23.82 | L | 0 |
| | ATOM | 572 | CG2 THR L | 72 | 29.542 | | 103.030 | 1.00 15.82 | L | С |
| 25 | MOTA | 573 | N LEU L | 73 | 26.493 | 15.457 | 99.807 | 1.00 19.72 | L | N |
| | ATOM | 574 | CA LEU L C LEU L | 73 73 | 26.030 26.217 | 16.236 17.677 | 98.663 99.201 | 1.00 16.55 1.00 14.66 | L L | C |
| | MOTA MOTA | 575 576 | C LEU L | 73 73 | 25.783 | | 100.322 | 1.00 14.00 | L | ŏ |
| | MOTA | 577 | CB LEU L | 73 | 24.513 | 15.996 | 98.415 | 1.00 12.04 | L | C |
| 30 | ATOM | 578 | CG LEU L | 73 | 23.862 | 16.933 | 97.412 | 1.00 15.16 | L | C |
| | MOTA | 579 | CD1 LEU L | 73 | 24.364 | 16.622 | 95.971 | 1.00 7.12 | L | C |
| | ATOM | 580 | CD2 LEU L | 73 | 22.333 26.779 | 16.778 18.549 | 97.425 98.366 | 1.00 10.12 1.00 15.06 | L L | N C |
| | ATOM ATOM | 581 582 | N THR L | 74 74 | 27.001 | 19.931 | 98.745 | 1.00 14.50 | L | Ĉ |
| 35 | MOTA | 583 | C THR L | 74 | 26.271 | 20.792 | 97.744 | 1.00 16.15 | L | C |
| | MOTA | 584 | O THR L | 74 | 26.297 | 20.513 | 96.532 | 1.00 20.55 | L | 0 |
| | ATOM | 585 | CB THR L | 74 | 28.497 | 20.274 | 98.756 | 1.00 14.01 | L | C |
| | ATOM | 586 | OG1 THR L | 74 | 29.136 28.719 | 19.508 21.793 | 99.777 99.068 | 1.00 10.91 1.00 8.51 | L L | C O |
| 40 | ATOM ATOM | 587 588 | CG2 THR L N ILE L | 74 75 | 25.520 | 21.784 | 98.233 | 1.00 16.30 | r r | N |
| 40 | ATOM | 589 | CA ILE L | 75 | 24.842 | 22.717 | 97.352 | 1.00 16.67 | L | C |
| | ATOM | 590 | C ILE L | 75 | 25.515 | 24.052 | 97.687 | 1.00 20.52 | L | C |
| | MOTA | 591 | O ILE L | 75 | 25.481 | 24.501 | 98.855 | 1.00 21.73 | ŗ | 0 |
| 4= | ATOM | 592 | CB ILE L | 75 75 | 23.331 22.756 | 22.809 21.387 | 97.656 97.597 | 1.00 20.98 1.00 14.60 | L L | C |
| 45 | MOTA MOTA | 593 594 | CG1 ILE L CG2 ILE L | 75 75 | 22.643 | 23.703 | 96.641 | 1.00 14.00 | L | č |
| | ATOM | 595 | CD1 ILE L | 75 | 21.239 | 21.348 | 97.963 | 1.00 10.72 | L | C |
| | ATOM | 596 | N ASN L | 76 | 26.085 | 24.703 | 96.691 | 1.00 18.75 | L | N |
| | MOTA | 597 | CA ASN L | 76 | 26.803 | 25.941 | 97.025 | 1.00 18.83 | L | C |
| 50 | MOTA | 598 | C ASN L | 76 76 | 27.022 27.640 | 26.797 26.378 | 95.789 94.829 | 1.00 19.14 1.00 20.66 | L L | O C |
| | MOTA MOTA | 599 600 | O ASN L CB ASN L | 76 | 28.159 | 25.535 | 97.655 | 1.00 20.07 | L | Č |
| | MOTA | 601 | CG ASN L | 76 | 28.920 | 26.738 | 98.205 | 1.00 20.61 | L | C |
| | MOTA | 602 | OD1 ASN L | 76 | 28.302 | 27.682 | 98.681 | 1.00 20.96 | L | 0 |
| 55 | MOTA | 603 | ND2 ASN L | 76 | 30.244 | 26.690 | 98.175 | 1.00 25.64 | ŗ | N |
| | MOTA | 604 | N PRO L | 77 | 26.467 25.632 | 28.005 28.644 | 95.757 96.793 | 1.00 22.23 1.00 22.24 | L L | C N |
| | MOTA MOTA | 605 606 | CA PRO L C PRO L | 77 77 | 24.205 | 28.126 | 96.665 | 1.00 22.29 | L | Č |
| | ATOM | 607 | O PRO L | 77 | 23.721 | 27.852 | 95.567 | 1.00 23.37 | L | 0 |
| 60 | ATOM | 608 | CB PRO L | 77 | 25.651 | 30.135 | 96.414 | 1.00 20.03 | L | C |
| | MOTA | 609 | CG PRO L | 77 | 25.601 | 30.058 | 94.807 | 1.00 18.01 | L | C |
| | ATOM | 610 | CD PRO L | 77 | 26.621 | 28.854 | 94.560 97.794 | 1.00 19.60 1.00 19.30 | L L | C N |
| | MOTA MOTA | 611 612 | N VAL L CA VAL L | 78 78 | 23.516 22.086 | 28.051 27.650 | 97.794 | 1.00 15.86 | L | C |
| 65 | MOTA | 613 | C VAL L | 78 | 21.237 | 28.809 | 97.198 | 1.00 15.02 | L | С |
| | ATOM | 614 | O VAL L | 78 | 21.528 | 30.006 | 97.458 | 1.00 18.62 | L | 0 |
| | MOTA | 615 | CB VAL L | 78 | 21.659 | 27.342 | 99.240 | 1.00 10.76 | L | C |
| | ATOM | 616 | CG1 VAL L | 78 | 20.108 | 27.338 | 99.344 99.691 | 1.00 15.65 1.00 8.70 | L L | C |
| | MOTA | 617 | CG2 VAL L | 78 | 22.225 | 25.962 | 22.02L | 1.00 0.70 | | C |

| | ATOM | 618 | n glu | L 79 | | 20.229 | 28.482 | 96.385 | 1.00 15.66 | L | N |
|-----|--------------|------------|--------------------|--------|------------------|------------------|------------------|--------------------|--------------------------|--------|--------|
| | MOTA | 619 | CA GLU | ь 79 | | 19.303 | 29.452 | 95.777 | 1.00 15.48 1.00 19.00 | L L | C |
| | ATOM | | C GLU | | | 17.890 17.679 | 29.108 28.011 | 96.280 96.728 | 1.00 19.00 1.00 18.75 | L L | Ö |
| 5 | MOTA MOTA | | CB GLU | | | 19.341 | 29.354 | 94.257 | 1.00 16.52 | L | C |
| Ū | ATOM | 623 | CG GLU | ь 79 |) | 20.703 | 29.701 | 93.731 | 1.00 17.33 | Ŀ | C |
| | ATOM | | CD GLU | | | 20.771 21.811 | 29.892 30.362 | 92.198 91.749 | 1.00 31.97 1.00 36.07 | L L | C |
| | MOTA MOTA | | OE1 GLU OE2 GLU | | | 19.829 | 29.549 | 91.476 | 1.00 19.91 | L | ŏ |
| 10 | ATOM | | N ALA | | | 16.946 | 30.041 | 96.179 | 1.00 17.42 | L | N |
| 10 | ATOM | | CA ALA | | | 15.594 | 29.804 | 96.728 | 1.00 15.69 | L | C |
| | MOTA | | C ALA | | | 14.941 | 28.596 | 96.125 | 1.00 17.37 | L | C |
| | MOTA | | O ALA | | | 14.202 14.655 | 27.902 31.034 | 96.797 96.432 | 1.00 20.28 1.00 17.81 | L L | C |
| 4.5 | ATOM ATOM | | CB ALA N ASP | | | 15.181 | 28.374 | 94.839 | 1.00 17.01 | L | N |
| 15 | MOTA | | CA ASP | _ | | 14.492 | 27.254 | 94.184 | 1.00 20.13 | L | C |
| | ATOM | | C ASP | L 8: | | 15.083 | 25.903 | 94.533 | 1.00 18.90 | L | C |
| | ATOM | 635 | O ASP | | | 14.614 | 24.889 | 93.991 | 1.00 22.61 | Ŀ | O C |
| | MOTA | 636 | CB ASP | | | 14.467 13.575 | 27.444 26.430 | 92.658 91.938 | 1.00 20.21 1.00 34.87 | L L | Č |
| 20 | MOTA | 637 638 | CG ASP OD1 ASP | | | 12.398 | 26.284 | 92.319 | 1.00 48.81 | L | ŏ |
| | ATOM ATOM | 639 | OD1 ASP | | | 14.054 | 25.764 | 90.982 | 1.00 50.24 | L | 0 |
| | MOTA | 640 | N ASP | | | 16.057 | 25.871 | 95.453 | 1.00 16.98 | L | N |
| | MOTA | 641 | CA ASP | | | 16.640 | 24.587 | 95.887 | 1.00 15.01 | L L | C |
| 25 | ATOM | 642 | C ASP | | | 15.839 16.144 | 23.921 22.779 | 97.038 97.470 | 1.00 15.72 1.00 19.30 | L | ŏ |
| | MOTA MOTA | 643 644 | O ASP CB ASP | | | 18.088 | 24.761 | 96.328 | 1.00 13.58 | L | C |
| | ATOM | 645 | CG ASP | | | 19.016 | 25.236 | 95.161 | 1.00 19.81 | L | C |
| | ATOM | 646 | OD1 ASP | г 8 | 2 | 18.685 | 25.119 | 93.925 | 1.00 15.99 | L | 0 |
| 30 | MOTA | 647 | OD2 ASP | | | 20.081 | 25.777 | 95.531 97.553 | 1.00 22.54 1.00 15.10 | L L | O N |
| | MOTA | 648 | N VAL | | | 14.810 14.008 | 24.609 23.957 | 98.617 | 1.00 13.10 | L | Ĉ |
| | ATOM ATOM | 649 650 | CA VAL | | | 13.427 | 22.662 | 98.020 | 1.00 17.36 | L | C |
| | ATOM | 651 | O VAL | | | 12.820 | 22.650 | 96.948 | 1.00 17.48 | L | 0 |
| 35 | MOTA | 652 | CB VAL | r 8 | 3 | 12.914 | 24.905 | 99.174 | 1.00 15.94 | ŗ | C |
| | ATOM | 653 | CG1 VAL | | | 13.604 | 25.942 | 100.046 | 1.00 23.49 1.00 25.18 | L L | C |
| | ATOM | 654 | CG2 VAL | | | 12.227 13.651 | 25.582 21.576 | 98.130 98.738 | 1.00 25.18 1.00 15.63 | L | N |
| | ATOM ATOM | 655 656 | N ALA | | 4 | 13.272 | 20.269 | 98.218 | 1.00 14.84 | r L | C |
| 40 | ATOM | 657 | C ALA | _ | $\overline{4}$ | 13.732 | 19.240 | 99.214 | 1.00 15.55 | L | C |
| | MOTA | 658 | O ALA | | 4 | 14.336 | 19.576 | 100.253 | 1.00 15.84 | L | 0 |
| | ATOM | 659 | CB ALA | | 4 | 14.071 | 20.056 17.959 | 96.900 98.930 | 1.00 14.40 1.00 15.71 | L L | C N |
| | MOTA | 660 661 | N THR | | 5 5 | 13.416 13.960 | 16.888 | 99.739 | 1.00 15.45 | L | Ĉ |
| 45 | ATOM ATOM | 662 | C THR | | 5 | 15.005 | 16.210 | 98.843 | 1.00 15.12 | L | С |
| -10 | MOTA | 663 | O THR | L 8 | 5 | 14.727 | 15.967 | 97.667 | 1.00 15.93 | L | 0 |
| | ATOM | 664 | CB THR | | 5 | 12.845 | 15.855 | 100.140 | 1.00 17.03 | L L | C O |
| | ATOM | 665 | OG1 THR | | 5 5 | 11.920 13.470 | 14.657 | 101.021 100.918 | 1.00 22.01 1.00 8.72 | L | č |
| 50 | MOTA MOTA | 666 667 | CG2 THR | | 6 | 16.183 | 15.916 | 99.411 | 1.00 14.04 | L | N |
| 50 | ATOM | 668 | CA TYR | | 6 | 17.268 | 15.309 | 98.667 | 1.00 13.13 | L | C |
| | MOTA | 669 | C TYP | E L S | 6 | 17.447 | 13.879 | 99.156 | 1.00 16.69 | L | С |
| | MOTA | 670 | O TYP | | 6 | 17.458 | 13.637 16.109 | 100.330 98.896 | 1.00 18.94 1.00 11.97 | L L | O C |
| EE | MOTA | 671 672 | CB TYF | | 6 | 18.564 18.443 | 17.491 | 98.305 | 1.00 11.60 | L | č |
| 55 | MOTA MOTA | 673 | CD1 TYF | | 6 | 17.811 | 18.516 | 98.981 | 1.00 7.53 | L | C |
| | MOTA | 674 | CD2 TYF | 3 L. S | 6 | 18.872 | 17.734 | 97.006 | 1.00 12.00 | L | C |
| | ATOM | 675 | CE1 TYF | | 6 | 17.590 | 19.772 | 98.364 | 1.00 11.09 | L | C |
| | ATOM | 676 | CE2 TYP | | 6 | 18.678 | 18.955 19.968 | 96.389 97.056 | 1.00 11.34 1.00 17.23 | L L | C |
| 60 | ATOM | 677 678 | OH TYP | | 16 16 | 18.043 17.888 | 21.177 | 96.447 | 1.00 17.23 | L | ŏ |
| | MOTA MOTA | 679 | N TYP | | 37 | 17.559 | 12.936 | 98.214 | 1.00 16.92 | L | N |
| | ATOM | 680 | CA TYP | ιь 8 | 37 | 17.721 | 11.533 | 98.587 | 1.00 13.58 | Ŀ | C |
| | MOTA | 681 | C TYI | 7 L, 8 | 37 | 19.002 | 10.935 | | 1.00 12.86 | L L | O C |
| 65 | ATOM | 682 | O TY | | 37 37 | 19.326 16.618 | 11.195 10.684 | | 1.00 18.14 1.00 6.47 | L | C |
| | MOTA MOTA | 683 684 | CB TYI | | 3 <i>1</i> 37 | 15.235 | 11.018 | | 1.00 18.98 | Ĺ | C |
| | MOTA | 685 | CD1 TY | | 37 | 14.461 | 11.985 | 97.824 | 1.00 11.56 | Ŀ | C |
| | ATOM | 686 | CD2 TY | яь а | 37 | 14.684 | 10.318 | 99.518 | 1.00 14.13 | L | С |
| | | | | | | 100 | | | | | |

| | 2001 | 607 | and | DISTEN T | 07 | 12 150 | 10 000 | 00 046 | 1 00 15 50 | - | ~ |
|-----------|-----------------|-----|------------------|------------------------|----|--------|--------|---------|------------|------------|------|
| | MOTA | 687 | CE1 | TYR L | 87 | 13.156 | 12.228 | 98.246 | 1.00 15.50 | L | C |
| | MOTA | 688 | CE2 | TYR L | 87 | 13.358 | 10.572 | 99.941 | 1.00 7.09 | L | C |
| | - | | | | | | | | | | |
| | ATOM | 689 | CZ | TYR L | 87 | 12.621 | 11.510 | 99.306 | 1.00 17.61 | L | C |
| | ATOM | 690 | OH | TYR L | 87 | 11.313 | 11.799 | 99.716 | 1.00 18.17 | I. | |
| _ | | | | | | | | | | | |
| 5 | MOTA | 691 | \mathbf{N} | CYS L | 88 | 19.673 | 10.099 | 98.850 | 1.00 9.84 | L | N |
| | MOTA | 692 | CA | CYS L | 88 | 20.813 | 9.367 | 98.272 | 1.00 14.40 | I | |
| | | | | | | | | | | | _ |
| | ATOM | 693 | С | CYS L | 88 | 20.235 | 7.961 | 97.902 | 1.00 15.10 | · <u>T</u> | , C |
| | | | | | | | | | | | |
| | ATOM | 694 | 0 | CYS L | 88 | 19.136 | 7.592 | 98.357 | 1.00 18.42 | L | . 0 |
| | MOTA | 695 | CB | CYS L | 88 | 21.962 | 9.241 | 99.263 | 1.00 12.72 | L | C |
| | | | | | | | | | | | |
| 10 | \mathbf{ATOM} | 696 | sg | CYS L | 88 | 21.464 | 8.575 | 100.910 | 1.00 16.04 | I | S |
| | ATOM | 697 | N | GLN L | 89 | 20.944 | 7.220 | 97.041 | 1.00 11.35 | I | |
| | ATOM | | TA | רד אזרדי | 09 | 20.544 | | | | 1. | |
| | ATOM | 698 | $^{\rm CA}$ | GLNL | 89 | 20.468 | 5.917 | 96.588 | 1.00 9.96 | L | C |
| | | | | | | | | | | | |
| | MOTA | 699 | С | GLN L | 89 | 21.692 | 5.101 | 96.156 | 1.00 13.56 | L | C |
| | MOTA | 700 | 0 | GLN L | 89 | 22,591 | 5.652 | 95.507 | 1.00 14.17 | L | |
| | | | | | | | | | | | |
| 15 | ATOM | 701 | CB | GLN L | 89 | 19.561 | 6.138 | 95.392 | 1.00 9.47 | L | C |
| | MOTA | 702 | CG | GLN L | 89 | 18.988 | 4.858 | 94.748 | 1.00 8.43 | L | |
| | | | | | | | | | | | |
| | MOTA | 703 | $^{\rm CD}$ | $\operatorname{GLN} L$ | 89 | 19.713 | 4.527 | 93.433 | 1.00 12.81 | L | C |
| | | | | | | | | | | | |
| | ATOM | 704 | OE1 | GLN L | 89 | 19.766 | 5.348 | 92.490 | 1.00 13.05 | I | 0 |
| | ATOM | 705 | NE2 | GLN L | 89 | 20.250 | 3.310 | 93.364 | 1.00 7.99 | L | N |
| | | | | | | | | | | | |
| 20 | ATOM | 706 | N | GLN L | 90 | 21.744 | 3.825 | 96.542 | 1.00 12.73 | L | N |
| | MOTA | 707 | CA | GLN L | 90 | 22.913 | 2.994 | 96.196 | 1.00 11.36 | L | |
| | | | | | | | | | | | |
| | ATOM | 708 | С | GLN L | 90 | 22.517 | 1.939 | 95.194 | 1.00 12.24 | L | C |
| | | 709 | 0 | GLN L | 90 | 21.399 | 1.436 | 95.209 | 1.00 8.64 | I | |
| | MOTA | | | | | | | | | 1. | |
| | MOTA | 710 | CB | GLN L | 90 | 23.527 | 2.285 | 97.415 | 1.00 9.81 | L | C |
| 05 | | | | | | | | | | | . ~ |
| 25 | ATOM | 711 | CG | GLN L | 90 | 22.598 | 1.298 | 98.110 | 1.00 14.99 | L | C |
| | MOTA | 712 | CD | GLN L | 90 | 22.598 | -0.129 | 97.521 | 1.00 18.05 | L | C |
| | | | | | | | | | | | |
| | MOTA | 713 | OE1 | GLN L | 90 | 23.545 | -0.566 | 96.864 | 1.00 15.88 | L | . 0 |
| | MOTA | 714 | NE2 | GLN L | 90 | 21.518 | -0.858 | 97.800 | 1.00 20.57 | L | |
| | | | | | | | | | | | |
| | ATOM | 715 | N | SER L | 91 | 23.473 | 1.641 | 94.322 | 1.00 13.95 | L | N |
| 00 | | | | | | | | | | | |
| 30 | MOTA | 716 | $^{\rm CA}$ | SER L | 91 | 23.290 | 0.693 | 93.251 | 1.00 19.79 | L | |
| | MOTA | 717 | C | SER L | 91 | 24.352 | -0.403 | 93.325 | 1.00 18.67 | L | C |
| | | | | | | | | | | | |
| | MOTA | 718 | 0 | SER L | 91 | 24.611 | -1.040 | 92.298 | 1.00 19.36 | L | . 0 |
| | ATOM | 719 | CB | SER L | 91 | 23.441 | 1.425 | 91.887 | 1.00 15.12 | L | |
| | | | | | | | | | | | |
| | MOTA | 720 | OG | SER L | 91 | 22.237 | 2.067 | 91.586 | 1.00 33.42 | L | . 0 |
| 25 | | | | | | | | | | | |
| 35 | MOTA | 721 | N | ASN L | 92 | 24.930 | -0.634 | 94.510 | 1.00 16.12 | L | |
| | ATOM | 722 | $^{\rm CA}$ | ASN L | 92 | 25.989 | -1.659 | 94.620 | 1.00 15.63 | L | C |
| | | | | | | | | | | | |
| | ATOM | 723 | С | ASN L | 92 | 25.422 | -3.053 | 94.890 | 1.00 14.30 | L | C |
| | MOTA | 724 | 0 | ASN L | 92 | 26.015 | -4.064 | 94.460 | 1.00 16.71 | L | |
| | | | | | | | | | | | |
| | MOTA | 725 | CB | ASN L | 92 | 27.040 | -1.288 | 95.676 | 1.00 15.71 | L | C |
| 40 | | | | | | | | | | | |
| 40 | MOTA | 726 | CG | ASN L | 92 | 28.307 | -2.149 | 95.545 | 1.00 14.45 | L | C |
| | MOTA | 727 | OD1 | ASN L | 92 | 28.831 | -2.324 | 94.450 | 1.00 27.57 | L | . 0 |
| | | | | | | | | | | | |
| | MOTA | 728 | ND2 | ASN L | 92 | 28.770 | -2.700 | 96.656 | 1.00 25.93 | L | , N |
| | MOTA | 729 | N | GLU L | 93 | 24.279 | ~3.143 | 95.562 | 1.00 16.66 | I | |
| | | | | | | | | | | | |
| | ATOM | 730 | $^{\mathrm{CA}}$ | GLU L | 93 | 23.643 | -4.433 | 95.783 | 1.00 16.68 | L | ı C |
| 45 | | 731 | | GLU L | 93 | 22.164 | -4.332 | 95.540 | | 7 | |
| 45 | MOTA | | C | | | | | | 1.00 18.74 | L | |
| | MOTA | 732 | 0 | GLU L | 93 | 21.542 | -3.325 | 95.804 | 1.00 20.03 | I | 0 |
| | | | | | | | | | | | |
| | ATOM | 733 | CB | GLU L | 93 | 23.772 | -4.934 | 97.261 | 1.00 20.26 | L | , C |
| | MOTA | 734 | CG | GLU L | 93 | 25.164 | ~5.095 | 97.612 | 1.00 24.66 | L | C |
| | | | | | | | | | | | |
| | MOTA | 735 | CD | GLU L | 93 | 25.373 | ~5.930 | 98.887 | 1.00 27.35 | L | |
| 50 | MOTA | 736 | OE1 | GLU L | 93 | 24.422 | -6.153 | 99.638 | 1.00 20.40 | I | . 0 |
| | | | | | | | | | | | |
| | ATOM | 737 | OE2 | GLU L | 93 | 26.517 | -6.309 | 99.032 | 1.00 31.57 | L | . 0 |
| | MOTA | 738 | N | ASP L | 94 | 21.584 | -5.438 | 95.123 | 1.00 20.63 | L | N |
| | | | | | | | | | | | 1 1/ |
| | MOTA | 739 | $^{\rm CA}$ | ASP L | 94 | 20.123 | -5.480 | 94.983 | 1.00 17.16 | I | C |
| | | | | | | | | | | | |
| | ATOM | 740 | С | ASP L | 94 | 19.620 | -5.956 | 96.366 | 1.00 16.50 | L | |
| 55 | MOTA | 741 | 0 | ASP L | 94 | 20.278 | -6.748 | 97.008 | 1.00 21.43 | L | . 0 |
| 00 | | | | | | | | | | | |
| | MOTA | 742 | CB | ASP L | 94 | 19.746 | -6.525 | 93.962 | 1.00 18.30 | L | C |
| | | 743 | CG | | 94 | 20.195 | ~6.159 | 92.573 | 1.00 22.97 | L | C |
| | ATOM | | | ASP L | | | | | | | |
| | ATOM | 744 | OD1 | ASP L | 94 | 20.453 | -4.967 | 92.336 | 1.00 31.49 | L | . 0 |
| | | | | | | | | | | | |
| | MOTA | 745 | OD2 | ASP L | 94 | 20.255 | -7.058 | 91.718 | 1.00 33.23 | L | |
| 60 | MOTA | 746 | N | PRO L | 95 | 18.473 | -5.447 | 96.836 | 1.00 18.36 | I | |
| 55 | | | | | | | | | | | |
| | ATOM | 747 | CA | PRO L | 95 | 17.663 | -4.449 | 96.112 | 1.00 15.59 | L | |
| | | 748 | | | | 18.313 | -3.067 | 96.210 | | I | Č |
| | ATOM | | С | PRO L | 95 | | | | 1.00 15.03 | | |
| | MOTA | 749 | 0 | PRO L | 95 | 18.880 | -2.731 | 97.243 | 1.00 15.51 | L | 0 |
| | | | | | | | | | | | ~ |
| | MOTA | 750 | CB | PRO L | 95 | 16.325 | -4.466 | 96.865 | 1.00 15.24 | L | C |
| 65 | ATOM | 751 | CG | PRO L | 95 | 16.748 | ~4.764 | 98.308 | 1.00 19.84 | L | |
| ~~ | | | | | | | | 00.000 | | | · ~ |
| | MOTA | 752 | $^{\rm CD}$ | PRO L | 95 | 17.832 | ~5.859 | 98.104 | 1.00 18.49 | L | |
| | MOTA | 753 | N | TRP L | 96 | 18.190 | -2.249 | 95.169 | 1.00 12.53 | L | |
| | | | | | | | | | | | |
| | ATOM | 754 | $^{\rm CA}$ | TRP L | 96 | 18.751 | -0.916 | 95.285 | 1.00 11.43 | L | C |
| | | 755 | C | TRP L | 96 | 17.888 | -0.227 | 96.339 | 1.00 15.42 | I | |
| | ATOM | 155 | C | 11/2 17 | 90 | 11.000 | -0.221 | 90.333 | T.00 TJ.47 | 1 | |
| | | | | | | | | | | | |

| | ATOM | 756 | 0 | TRP L | 96 | 16.668 | -0.463 | 96.364 | 1.00 | 16.13 | L | O |
|-----|--------------|------------|------------|----------------|------------|------------------|------------------|--------------------|-------------|----------------|--------------------|--------|
| | ATOM | 757 | СВ | TRP L | 96 | 18.596 | -0.141 | 93.994 | 1.00 | 6.29 | L L | č |
| | MOTA | 758 | CG | TRP L | 96 | 19.497 | -0.624 | 92.924 | 1.00 | 18.26 | L | C |
| _ | ATOM | 759 | CD1 | | 96 | 20.292 | -1.701 | 92.954 | 1.00 | 23.00 | L | C |
| 5 | MOTA | 760 | CD2 | TRP L | 96 96 | 19.694 | 0.007 | 91.657 | 1.00 | 15.27 | L | C |
| | ATOM ATOM | 761 762 | NE1 CE2 | TRP L | 96 96 | 21.009 20.650 | -1.785 -0.744 | 91.775 90.964 | 1.00 1.00 | 15.73 22.20 | L L | C N |
| | ATOM | 763 | CE3 | TRP L | 96 | 19.148 | 1.137 | 91.058 | | 13.08 | L L | C |
| | MOTA | 764 | CZ2 | TRP L | 96 | 21.092 | -0.397 | 89.681 | 1.00 | 23.50 | L | Č |
| 10 | ATOM | 765 | CZ3 | TRP L | 96 | 19.583 | 1.498 | 89.787 | 1.00 | | L | Č |
| | MOTA | 766 | CH2 | TRP L | 96 | 20.552 | 0.729 | 89.118 | 1.00 | 23.23 | L | C |
| | MOTA | 767 | N | THR L | 97 | 18.521 | 0.636 | 97.153 | 1.00 | 14.07 | L | N |
| | ATOM | 768 | CA | THR L | 97 | 17.784 | 1.306 | 98.212 | 1.00 | 14.31 | L | C |
| 4 - | MOTA | 769 | C | THR L | 97 | 18.051 | 2.804 | 98.229 97.707 | 1.00 | 16.18 | L | C |
| 15 | ATOM ATOM | 770 771 | O CB | THR L | 97 97 | 19.063 18.160 | 3.276 0.742 | 99.570 | 1.00 | 18.79 13.49 | L L | 0 |
| | ATOM | 772 | OG1 | | 97 | 19.588 | 0.742 | 99.618 | 1.00 | 17.28 | Ľ | Õ |
| | MOTA | 773 | CG2 | THR L | 97 | 17.561 | -0.728 | 99.749 | 1.00 | 10.34 | L | Č |
| | ATOM | 774 | N | PHE L | 98 | 17.119 | 3.515 | 98.851 | 1.00 | 16.74 | \mathbf{L} | N |
| 20 | MOTA | 775 | CA | PHE L | 98 | 17.173 | 4.966 | 98.957 | 1.00 | 15.24 | L | C |
| | MOTA | 776 | C | PHE L | 98 | 17.292 | 5.386 | 100.417 | 1.00 | 14.99 | L | C |
| | ATOM | 777 | O | PHE L | 98 98 | 16.795 15.898 | 4.676 5.572 | 101.313 98.435 | | 13.01 | L | 0 |
| | MOTA MOTA | 778 779 | CB CG | PHE L | 98 98 | 15.898 | 5.522 | 96.435 | 1.00 1.00 | 12.91 13.58 | L L | C |
| 25 | MOTA | 780 | | PHE L | 98 | 15.204 | 4.390 | 96.335 | 1.00 | 11.52 | L | č |
| | ATOM | 781 | | PHE L | 98 | 16.004 | 6.648 | 96.173 | 1.00 | 10.32 | L | Č |
| | MOTA | 782 | CE1 | PHE L | 98 | 14.981 | 4.388 | 94.966 | 1.00 | 10.75 | L | C |
| | ATOM | 783 | CE2 | | 98 | 15.770 | 6.644 | 94.808 | 1.00 | 13.28 | L | C |
| | ATOM | 784 | CZ | PHE L | 98 | 15.259 | 5.503 | 94.217 | | 15.23 | L | C |
| 30 | ATOM | 785 | N | GLY L | 99 99 | 17.984 18.027 | 6.511 7.055 | 100.661 | 1.00 1.00 | 13.55 10.54 | L L | N |
| | MOTA MOTA | 786 787 | CA C | GLY L | 99 | 16.637 | 7.610 | 102.027 102.318 | 1.00 | 12.58 | F F | C |
| | ATOM | 788 | Ö | GLY L | 99 | 15.796 | 7.735 | 101.424 | 1.00 | 9.94 | L | ŏ |
| | ATOM | 789 | N | | 100 | 16.424 | 8.022 | 103.565 | 1.00 | 12.36 | L | N |
| 35 | ATOM | 790 | CA | GLY L | 100 | 15.147 | 8.553 | 103.982 | 1.00 | 8.70 | L | C |
| | MOTA | 791 | С | GLY L | 100 | 14.891 | | 103.583 | | 15.60 | L | C |
| | ATOM | 792 | 0 | GLY L | 100 | 13.803 | 10.533 | 103.828 | 1.00 | 17.49 | L | 0 |
| | MOTA | 793 | N | | 101 | 15.910 | 10.695 | 103.040 | 1.00 | 15.34 | $\bar{\mathbf{r}}$ | N |
| 40 | ATOM ATOM | 794 795 | CA C | GLY L | 101 101 | 15.662 16.100 | 12.053 13.108 | 102.574 103.567 | 1.00 | 18.81 17.29 | L L | C |
| 40 | ATOM | 796 | Ö | GLY L | 101 | 16.100 | 12.868 | 104.775 | 1.00 | 18.50 | L | õ |
| | ATOM | 797 | Ŋ | THR L | 102 | 16.577 | 14.239 | 103.050 | 1.00 | 15.70 | L | N |
| | MOTA | 798 | CA | THR L | 102 | 16.963 | 15.383 | 103.902 | 1.00 | 13.96 | L | C |
| | ATOM | 799 | С | THR L | | 16.243 | 16.556 | 103.300 | 1.00 | 12.46 | L | C |
| 45 | ATOM | 800 | 0 | THR L | | 16.358 | | 102.080 | 1.00 | 11.12 | L | 0 |
| | ATOM ATOM | 801 802 | CB OG1 | THR L | 102 | 18.526 19.194 | 15.654 14.618 | 103.915 104.653 | 1.00 | 13.19 18.45 | L L | C |
| | ATOM | 803 | CG2 | | | 18.813 | | 104.578 | 1.00 | 7.06 | P D | Č |
| | ATOM | 804 | N | LYS L | | 15.488 | | 104.130 | | 11.45 | L | Ŋ |
| 50 | MOTA | 805 | CA | LYS L | | 14.756 | | 103.615 | 1.00 | 13.95 | L | C |
| | ATOM | 806 | C | LYS L | | 15.578 | | 103.729 | | 12.14 | L | C |
| | MOTA | 807 | 0 | LYS L | | 16.098 | | 104.795 | | 16.90 | Ţ. | 0 |
| | ATOM | 808 | CB | LYS L | | 13.411 12.759 | | 104.360 103.933 | | 11.00 25.30 | L L | C |
| 55 | ATOM ATOM | 809 810 | CG CD | LYS L LYS L | | 11.185 | | 103.933 | | 32.62 | P D | C |
| 55 | ATOM | 811 | CE | LYS L | | 10.533 | | 105.063 | | 42.65 | L | Č |
| | ATOM | 812 | NZ | LYS L | | 9.000 | | 104.966 | | 51.76 | L | N |
| | MOTA | 813 | N | LEU L | | 15.689 | | 102.641 | | 11.40 | L | N |
| | MOTA | 814 | CA | LEU L | | 16.470 | | 102.700 | | 14.03 | L | C |
| 60 | ATOM | 815 | C | LEU L | | 15.472 | | 102.763 | | 16.12 | L | C |
| | ATOM | 816 | 0 | LEU L | | 14.494 | | 101.964 | | 19.86 | L | 0 |
| | ATOM ATOM | 817 818 | CB CG | LEU L | | 17.316 18.153 | | 101.444 101.382 | | 17.08 15.21 | L L | C |
| | ATOM | 819 | | LEU L | | 19.243 | | 101.362 | | 14.42 | L | C |
| 65 | MOTA | 820 | | LEU L | | 18.758 | 23.351 | 99.967 | | 21.88 | L | Č |
| | ATOM | 821 | N | GLU L | 105 | 15.738 | 23.838 | 103.669 | 1.00 | 19.74 | L | N |
| | MOTA | 822 | CA | GLU L | | 14.883 | | 103.776 | | 23.03 | Ŀ | C |
| | MOTA | 823 | C | GLU L | | 15.777 | | 103.798 | | 21.66 | Ŀ | C |
| | ATOM | 824 | 0 | GLU L | 102 | 16.995 | 26.152 | 104.094 | T.00 | 23.85 | P | 0 |

| | ATOM ATOM | 825 826 | CB | GLU L | 105 105 | | .058 .822 | 24.996 24.033 | 5 105.0 3 104.8 | | 1.00 | 20.70 42.64 | Ļ | C |
|----|--------------|------------|------------|----------------|------------|-----|--------------|------------------|--------------------|-----|------|----------------|---------|--------|
| | ATOM | 827 | CD | | 105 | | 991 | 23.732 | | | 1.00 | | L L | C |
| - | ATOM ATOM | 828 | OE1 | | 105 | | 550 | 23.403 | | | 1.00 | | L | 0 |
| 5 | ATOM | 829 830 | OE2 N | ILE L | 105 106 | | .772 .167 | 23.799 | 9 105.9 9 103.5 | | 1.00 | 35.54 19.49 | L L | O |
| | ATOM | 831 | ĈA | | 106 | | 897 | | 103.4 | | | 18.78 | T. | N C |
| | ATOM | 832 | C | ILE L | | 15. | 594 | 29.515 | | | | 18.92 | L | C |
| 10 | ATOM ATOM | 833 834 | O CB | | 106 106 | | 423 454 | 29.655 29.520 | | | | 17.74 | L | 0 |
| .0 | ATOM | 835 | | | 106 | | 651 | 28.723 | | | | 18.45 23.36 | L L | C |
| | MOTA | 836 | CG2 | ILE L | 106 | 16. | 165 | 30.884 | 102.2 | 287 | | 17.39 | L | č |
| | ATOM | 837 | | ILE L | | | 082 | | 100.7 | | | 11.46 | L | C |
| 15 | ATOM ATOM | 838 839 | N CA | LYS L LYS L | 107 | | 622 391 | 30.020 |) 105.3 ! 106.5 | | | 18.87 18.21 | L L | N |
| | MOTA | 840 | CB | LYS L | | | 507 | 30.812 | | | | 13.40 | L | C |
| | MOTA | 841 | C | | 107 | 16. | 341 | 32.312 | 105.9 | 53 | 1.00 | | L | č |
| | ATOM | 842 | 0 | LYS L | | | 316 | | 105.3 | | | 26.63 | L | 0 |
| 20 | ATOM ATOM | 843 844 | N CA | ARG L ARG L | 108 | | 208 | 34.375 | . 106.0 5 105.5 | | 1.00 | 24.68 23.09 | L L | C N |
| | MOTA | 845 | C | | 108 | | 597 | 35.310 | | | 1.00 | | L | C |
| | MOTA | 846 | 0 | ARG L | | 14. | 547 | 34.974 | 107.8 | | 1.00 | | L | 0 |
| | MOTA MOTA | 847 848 | CB CG | ARG L | | | 151 | | 104.3 | | | 19.08 | Ŀ | C |
| 25 | MOTA | | CD | ARG L ARG L | 108 108 | | 735 672 | 33.971 34.639 | | | 1.00 | 22.27 21.24 | L L | C |
| | ATOM | 850 | NE | | 108 | | 420 | 36.012 | _ | | 1.00 | | L | И |
| | ATOM | 851 | CZ | ARG L | | | 862 | 36.858 | | | 1.00 | | L | C |
| | MOTA MOTA | 852 853 | NH1 NH2 | | | | 555 614 | 36.441 38.120 | | - | 1.00 | | L | И |
| 30 | MOTA | 854 | N | ALA L | | | 245 | 36.539 | | | | 20.00 22.10 | L L | N |
| | MOTA | 855 | CA | ALA L | 109 | 13. | 729 | 37.503 | | | 1.00 | | r | C |
| | ATOM | 856 | C | ALA L | | | 312 | 37.142 | | | | 28.19 | L | C |
| | MOTA MOTA | 857 858 | O CB | ALA L ALA L | | | 497 730 | 36.641 38.883 | | | 1.00 | 28.86 19.28 | L | 0 |
| 35 | MOTA | 859 | N | ASP L | | | 904 | 37.545 | | | | 24.17 | L L | N C |
| | MOTA | 860 | CA | ASP L | 110 | | 526 | | 109.2 | 94 | 1.00 | 21.56 | L | Č |
| | MOTA | 861 | C | ASP L | | | 516 | 37.934 | | | | 23.66 | L | C |
| | MOTA MOTA | 862 863 | O CB | ASP L ASP L | | | 784 297 | 39.005 | 107.8 110.6 | | 1.00 | 22.76 19.33 | L L | 0 |
| 40 | ATOM | 864 | CG | ASP L | | | 020 | 37.003 | | | 1.00 | | L L | G |
| | MOTA | 865 | | ASP L | | 11. | 593 | 35.921 | 111.4 | 58 | 1.00 | 25.30 | L | ŏ |
| | MOTA MOTA | 866 867 | | ASP L ALA L | | | 969 | | 112.9 | | | 38.99 | L | 0 |
| | ATOM | 868 | N CA | ALA L | | | 357 330 | 37.305 | 108.1 | | | 21.57 17.99 | L L | C M |
| 15 | MOTA | 869 | C | ALA L | | | 960 | 37.587 | | | | 20.07 | L | ç |
| | MOTA | 870 | 0 | ALA L | | | 625 | | 108.1 | .63 | 1.00 | 22.24 | L | 0 |
| | MOTA MOTA | 871 872 | CB N | ALA L ALA L | | | 398 147 | | 105.8 108.1 | | | 11.33 | L | C |
| | ATOM | 873 | CA | ALA L | | | 860 | | 108.7 | | | 18.94 18.42 | L L | C N |
| 50 | MOTA | 874 | C | ALA L | 112 | | 873 | | 107.8 | | | 20.56 | L | C |
| | ATOM | 875 | 0 | ALA L | | | 869 | | 106.6 | | | 25.17 | L | 0 |
| | MOTA MOTA | 876 877 | CB N | ALA L PRO L | | | 221 957 | | 109.3 | | | 15.77 19.48 | Ļ | C |
| | ATOM | 878 | CA | PRO L | | | 994 | | 107.4 | | | 17.01 | L L | C N |
| 55 | MOTA | 879 | C | PRO L | 113 | -0. | 051 | 37.193 | 106.8 | 95 | | 17.50 | L | č |
| | ATOM | 880 | 0 | PRO L | | | 427 | | 107.5 | | | 21.67 | L | 0 |
| | MOTA ATOM | 881 882 | CB CG | PRO L PRO L | | | 352 478 | | 108.2° | | | 16.83 10.92 | L | C |
| | MOTA | 883 | CD | PRO L | | | 853 | | 109.6 | | | 17.62 | L L | G G |
| 30 | ATOM | 884 | N | THR L | 114 | -0. | 511 | 36.947 | 105.6 | 79 | 1.00 | 21.82 | L | N |
| | ATOM | 885 886 | CA | THR L | | | 625 | | 105.1 | | | 21.62 | ŗ | C |
| | ATOM ATOM | 886 887 | C O | THR L THR L | | | 839 946 | | 105.3 104.7 | | | 24.80 25.84 | L L | C |
| | ATOM | 888 | CB | THR L | | | 439 | | 104.7 | | | 24.03 | T Tr | С О |
| 35 | ATOM | 889 | OG1 | THR L | 114 | -0. | 309 | 38.827 | 103.4 | 60 | 1.00 | 25.12 | L | 0 |
| | ATOM | 890 891 | CG2 | | | | 655 | 38.604 | | | | 15.64 | Ļ | C |
| | ATOM ATOM | 891 892 | N CA | VAL L VAL L | | | 752 897 | | 106.25 106.65 | | | 22.00 21.60 | L L | C N |
| | ATOM | 893 | C | VAL L | | | 170 | | 105.94 | | | 23.51 | L | G |
| | | | | | | | | | | | | | | |

| | ATOM ATOM ATOM | 894 895 896 | O CB CG1 | VAL L VAL L VAL L | 115 115 115 | -6.455 -5.104 -6.171 | | L05.906 L08.159 L08.620 | 1.00 | 22.67 18.30 18.51 | L L L | 000 |
|----|----------------------|-------------------|----------------|-------------------------|-------------------|----------------------------|----------------------|-------------------------------|------|-------------------------|----------------------|---------------|
| _ | ATOM | 897 | | VAL L | 115 | -3.743 | 36.262 1 | L08.930 | 1.00 | 15.64 | L | C |
| 5 | MOTA MOTA | 898 899 | N CA | SER L SER L | | -6.920 -8.177 | 35.878 1 36.131 1 | 105.413 | 1.00 | 21.18 19.67 | Ŀ | N |
| | ATOM | 900 | C | SER L | | -9.200 | | 104.073 | 1.00 | | L L | C |
| | MOTA | 901 | 0 | SER L | | -8.878 | 33.963 1 | .05.281 | 1.00 | 19.14 | L | 0 |
| 10 | ATOM ATOM | 902 903 | CB OG | SER L SER L | | -8.003 -6.991 | 35.930 1 36.777 1 | | | 16.47 | $\tilde{\mathbf{r}}$ | C |
| 10 | ATOM | 904 | И | ILE L | | -10.438 | | L02.687 L05.478 | | 31.49 18.42 | L L | N O |
| | MOTA | 905 | CA | ILE L | 117 | -11.452 | 34.627 1 | .05.968 | 1.00 | 19.19 | L | Ĉ |
| | MOTA | 906 907 | C | ILE L | | -12.594 | 34.564 1 | | | 18.21 | Ŀ | C |
| 15 | ATOM ATOM | 908 | O CB | ILE P | | -12.884 -11.980 | 35.572 1 35.028 1 | 104.306 107.384 | 1.00 | | L L | C |
| | ATOM | 909 | CG1 | ILE L | 117 | -12.950 | 33.964 1 | | | 16.18 | L | Č |
| | MOTA | 910 | CG2 | | | -12.633 | 36.421 1 | | 1.00 | | L | C |
| | ATOM ATOM | 911 912 | CD1 N | | 117 118 | -13.317 -13.211 | | .09.365 .04.839 | 1.00 | 21.53 16.84 | L L | C N |
| 20 | MOTA | 913 | ĈA | PHE L | | -14.262 | 33.214 1 | | 1.00 | | L | C |
| | MOTA | 914 | C | PHE L | | -15.490 | 32.512 1 | 04.373 | | 19.74 | L | C |
| | ATOM ATOM | 915 916 | O CB | PHE L | 118 | -15.406 -13.776 | 31.427 1 32.382 1 | .04.918 | 1.00 | 24.08 | L | 0 |
| | MOTA | 917 | CG | PHE L | 118 | -12.558 | | 02.032 | | 16.32 19.49 | L L | C |
| 25 | MOTA | 918 | CD1 | PHE L | 118 | -11.308 | 32.634 1 | | | 23.15 | Ĺ | Č |
| | MOTA | 919 920 | CD2 | | 118 | -12.653 | | .00.964 | | 16.22 | Ŀ | C |
| | ATOM ATOM | 921 | CE1 CE2 | | | -10.145 -11.486 | 33.225 1 34.395 1 | .02.011 | | 27.60 18.98 | L L | C |
| | ATOM | 922 | CZ | PHE L | 118 | -10.252 | 34.104 1 | | 1.00 | 19.75 | r r | c |
| 30 | MOTA | 923 | N | PRO L | | -16.671 | 33.102 1 | | | 24.09 | L | N |
| | ATOM ATOM | 924 925 | CA C | PRO L | | -17.866 -18.187 | 32.401 1 31.236 1 | .04.643 | 1.00 | | L | C |
| | ATOM | 926 | Õ | | 119 | -17.649 | 31.105 1 | | | 22.99 25.33 | L L | C |
| | ATOM | 927 | CB | PRO L | 119 | -18.993 | 33.441 1 | | | 21.57 | L | Č |
| 35 | MOTA | 928 | CG | PRO L | | -18.289 | 34.768 1 | | | 24.58 | L | С |
| | ATOM ATOM | 929 930 | CD N | PRO L PRO L | | -16.957 -19.111 | | .03.742 | 1.00 | | L | C |
| | ATOM | 931 | CA | PRO L | | -19.548 | | .04.207 .03.454 | 1.00 | 24.97 20.35 | L L | С И |
| | MOTA | 932 | C | PRO L | 120 | -20.169 | 29.766 1 | .02.153 | | 22.34 | L | č |
| 40 | ATOM | 933 | 0 | PRO L | | -20.757 | | .02.165 | | 27.53 | L | 0 |
| | MOTA MOTA | 934 935 | CB CG | PRO L | | -20.626 -20.336 | | .04.336 .05.688 | 1.00 | 21.43 24.10 | L L | C |
| | ATOM | 936 | CD | PRO L | | -19.783 | | .05.534 | 1.00 | 26.50 | L | C |
| 45 | MOTA | 937 | N | SER L | | -20.021 | | .01.055 | | 26.13 | L | N |
| 45 | MOTA MOTA | 938 939 | , CA C | SER L SER L | | -20.559 -22.061 | | 99.739 | | 28.80 | L | C |
| | ATOM | 940 | Ö | SER L | | -22.508 | | 99.748 .00.482 | | 30.89 28.98 | L L | C |
| | MOTA | 941 | CB | SER L | 121 | -19.906 | | 98.591 | | 29.25 | Ĩ. | č |
| 50 | ATOM | 942 | OG | SER L | | -20.172 | | 98.686 | | 28.45 | L | 0 |
| 50 | MOTA MOTA | 943 944 | N CA | SER L SER L | | -22.831 -24.266 | | 98.916 98.862 | | 33.37 34.56 | L L | C N |
| | ATOM | 945 | C | SER L | | -24.432 | | 98.360 | | 30.86 | Ĺ | G |
| | MOTA | 946 | 0 | SER L | | -25.288 | 27.470 | 98.811 | | 31.28 | ${f L}$ | 0 |
| 55 | MOTA MOTA | 947 948 | CB OG | SER L SER L | | -24.935 -24.460 | | 97.903 96.600 | | 36.90 | Ţ. | C |
| - | ATOM | 949 | И | GLU L | | -23.571 | | 97.436 | | 48.86 28.18 | L L | N O |
| | MOTA | 950 | CA | GLU L | 123 | -23.659 | 26.408 | 96.936 | | 33.35 | L | C |
| | ATOM | 951 | C | GLU L | | -23.564 | | 98.042 | | 30.77 | L | C |
| 60 | MOTA MOTA | 952 953 | O CB | GLU L | | -24.316 -22.554 | | 98.049 95.913 | | 28.32 35.48 | L L | С О |
| | ATOM | 954 | ĊĠ | GLU L | | -22.812 | | 94.643 | | 49.39 | L | C |
| | MOTA | 955 | CD | GLU L | | -22.019 | 28.188 | 94.524 | | 60.63 | L | Č |
| | ATOM ATOM | 956 957 | OE1 OE2 | | | -22.009 | | 95.522 | | 60.83 | Ţ | 0 |
| 65 | ATOM | 957 958 | N N | GLU L GLN L | | -21.405 -22.619 | | 93.434 98.978 | | 60.19 30.73 | L L | И О |
| | MOTA | 959 | CA | GLN L | 124 | -22.495 | | 00.046 | | 27.46 | L | C. |
| | ATOM | 960 | C | GLN L | 124 | -23.678 | 24.587 1 | 01.005 | 1.00 | 25.19 | L | C |
| | MOTA MOTA | 961 962 | O CB | GLN L | | -24.172 | | 01.459 | | 25.43 | L | 0 |
| | 7 OI1 | J U Z | CD | GLN L | 404 | -21.142 | 24.693 1 | 00.82/ | T.00 | 28.38 | L | С |

| | MOTA | 0.63 | aa | OT N T 124 | | -21.002 | 02 700 101 0 | 200 | 1 00 17 60 | | |
|-----|-----------------|---------|---------|------------|---|---------|-----------------------|-----|---------------------------------------|---|--------------|
| | | 963 | CG | GLN L 124 | | | 23.700 101.9 | | 1.00 17.62 | L | С |
| | MOTA | 964 | CD | GLN L 124 | | -19.695 | 23.785 102.7 | 732 | 1.00 19.12 | L | C |
| | ATOM | 965 | OE1 | GLN L 124 | | -19.129 | 24.872 102.8 | | 1.00 20.58 | | |
| | | | | | | | | | | L | 0 |
| | MOTA | 966 | NE2 | GLN L 124 | | -19.218 | 22.628 103.2 | 260 | 1.00 14.19 | L | \mathbf{N} |
| 5 | ATOM | 967 | N | LEU L 125 | | -24.128 | 25.781 101.3 | 221 | 1.00 23.58 | L | N |
| • | | | | | | | | | | | |
| | MOTA | 968 | ca | LEU L 125 | | -25.255 | 25.923 102.2 | 446 | 1.00 26.99 | L | С |
| | ATOM | 969 | C | LEU L 125 | | -26.482 | 25.150 101.7 | 714 | 1.00 31.07 | L | С |
| | MOTA | 970 | | LEU L 125 | | | | | | | |
| | | | 0 | | | -27.160 | 24.439 102.4 | | 1.00 31.01 | L | 0 |
| | ATOM | 971 | CB | LEU L 125 | | -25.574 | 27.404 102.4 | 142 | 1.00 21.80 | L | C |
| 10 | ATOM | 972 | CG | LEU L 125 | | -24.497 | 28.130 103.2 | | | | ~ |
| 10 | | | | | | | | | 1.00 26.32 | L | C |
| | ATOM | 973 | CD1 | LEU L 125 | | -24.696 | 29.650 103.2 | 236 | 1.00 8.36 | L | C |
| | MOTA | 974 | CD3 | LEU L 125 | | -24.556 | 27.611 104.6 | | 1.00 20.84 | | |
| | | | | | | | | | | L | С |
| | MOTA | 975 | N | THR L 126 | | -26.753 | 25.264 100.4 | 124 | 1.00 33.07 | L | N |
| | ATOM | 976 | CA | THR L 126 | | -27.880 | 24.508 99.8 | 276 | 1.00 35.65 | L | |
| 4 | | | | | | | | | | | С |
| 15 | \mathbf{MOTA} | 977 | С | THR L 126 | | -27.736 | 22.993 100.1 | 109 | 1.00 38.92 | L | С |
| | ATOM | 978 | 0 | THR L 126 | | -28.733 | 22.282 100.0 | 141 | 1.00 45.16 | L | 0 |
| | | | | | | | | | | | |
| | ATOM | 979 | CB | THR L 126 | | -28.021 | 24.678 98.3 | 3/6 | 1.00 37.07 | L | C |
| | MOTA | 980 | OG1 | THR L 126 | | -26.987 | 23.913 97.7 | 745 | 1.00 49,44 | L | 0 |
| | MOTA | 981 | CG2 | THR L 126 | | -27.929 | | | | | |
| | | | | | | | | | 1.00 27.81 | L | C |
| 20 | ATOM | 982 | N | SER L 127 | | -26.517 | 22.483 100.3 | 366 | 1.00 38.10 | L | N |
| | MOTA | 983 | CA | SER L 127 | | -26.319 | 21.040 100.5 | | 1.00 34.68 | | |
| | | | | | | | | | | L | С |
| | ATOM | 984 | C | SER L 127 | | -26.420 | 20.705 102.0 |)55 | 1.00 34.07 | L | C |
| | MOTA | 985 | 0 | SER L 127 | | -26.321 | 19.533 102.4 | 178 | 1.00 39.83 | L | 0 |
| | | | | | | | | | | | |
| | ATOM | 986 | CB | SER L 127 | | -24.949 | 20.596 100.0 | J94 | 1.00 34.83 | L | C |
| 25 | ATOM | 987 | OG | SER L 127 | | -24.807 | 20.845 98.7 | 713 | 1.00 44.79 | Ľ | 0 |
| | MOTA | 988 | | | | -26.596 | | | | | |
| | | | N | GLY L 128 | | | 21.730 102.8 | | 1.00 29.72 | L | N |
| | ATOM | 989 | CA | GLY L 128 | | -26.717 | 21.469 104.2 | 259 | 1.00 34.23 | L | C |
| | MOTA | 990 | С | GLY L 128 | | -25.440 | 21,697 105.0 | 130 | 1.00 36.19 | L | |
| | | | | | | | | | · · · · · · · · · · · · · · · · · · · | | C |
| | ATOM | 991 | 0 | GLY L 128 | | -25.456 | 21.612 106.2 | 264 | 1.00 40.26 | L | 0 |
| 30 | MOTA | 992 | N | GLY L 129 | | -24.353 | 22.020 104.3 | 326 | 1.00 33.03 | L | N |
| | | | | | | | | | | | |
| | MOTA | 993 | CA | GLY L 129 | | -23.092 | 22.207 105.0 | 109 | 1.00 31.52 | L | C |
| | ATOM | 994 | С | GLY L 129 | | -22.632 | 23.635 105.1 | 01 | 1.00 30.69 | L | С |
| | | | | | | | | | | | |
| | MOTA | 995 | 0 | GLY L 129 | | -23.196 | 24.524 104.4 | 153 | 1.00 28.36 | L | O. |
| | ATOM | 996 | N | ALA L 130 | | -21.609 | 23.859 105.9 | 927 | 1.00 29.57 | L | N |
| 35 | | | | | | | | | | | |
| 30 | MOTA | 997 | CA | ALA L 130 | | -21.095 | 25.205 106.1 | 747 | 1.00 29.07 | L | С |
| | ATOM | 998 | С | ALA L 130 | | -19.650 | 25.164 106.5 | 583 | 1.00 27.65 | L | C |
| | MOTA | 999 | ō | ALA L 130 | | -19.376 | 25.016 107.7 | | | | |
| | | | | | | | | | 1.00 32.06 | L | 0 |
| | \mathbf{ATOM} | 1000 | CB | ALA L 130 | | -21.909 | 25.940 107.2 | 211 | 1.00 25.02 | L | С |
| | ATOM | 1001 | N | SER L 131 | | -18.732 | 25.329 105.6 | | | | |
| | | | | | | | | | 1.00 26.55 | L | И |
| 40 | ATOM | 1002 | CA | SER L 131 | | -17.320 | 25.336 105.9 | 98 | 1.00 23.33 | L | C |
| | MOTA | 1003 | C | SER L 131 | | -16.890 | 26.778 105.9 | 221 | 1.00 23.98 | L | Č |
| | | | | | | | | | | - | |
| | MOTA | 1004 | 0 | SER L 131 | | -17.229 | 27.504 104.9 | 148 | 1.00 27.26 | L | 0 |
| | ATOM | 1005 | CB | SER L 131 | | -16.504 | 24.489 105.0 | 005 | 1.00 18.37 | L | С |
| | | | | | | | | | | | |
| | MOTA | 1006 | OG | SER L 131 | | -16.912 | 23.139 105.0 | JUT | 1.00 24.81 | L | 0 |
| 45 | \mathbf{ATOM} | 1007 | N | VAL L 132 | | -16.156 | 27.213 106.9 | 955 | 1.00 20.02 | L | N |
| | ATOM | 1008 | CA | VAL L 132 | | -15.639 | 28.556 107.0 | | | | |
| | | | | | | | | | 1.00 22.56 | L | С |
| | MOTA | 1009 | C | VAL L 132 | | -14.114 | 28.368 106.8 | 324 | 1.00 19.29 | L | C |
| | MOTA | 1010 | 0 | VAL L 132 | | -13.500 | 27.522 107.5 | 500 | 1.00 17.72 | L | ō |
| | | | | | | | | | | | |
| | ATOM | 1011 | CB | VAL L 132 | | -15.862 | 29.175 108.4 | | 1.00 23.70 | L | C |
| 50 | ATOM | 1012 | CG1 | VAL L 132 | | -15.461 | 30.666 108.3 | 372 | 1.00 19.40 | L | С |
| | ATOM | 1013 | | VAL L 132 | | -17.369 | 29.077 108.8 | | 1.00 21.15 | | |
| | | | | | | | | | | L | С |
| | ATOM | 1014 | N | VAL L 133 | | -13.531 | 29.141 105.9 | 14 | 1.00 18.23 | L | N |
| | MOTA | 1015 | CA | VAL L 133 | | -12.110 | 28.959 105.5 | | 1.00 16.84 | L | C |
| | | | | | | | | | | | |
| | ATOM | 1016 | C | VAL L 133 | | -11.267 | 30.201 105.8 | 370 | 1.00 16.55 | L | C |
| 55 | MOTA | 1017 | 0 | VAL L 133 | | -11.670 | 31.324 105.6 | 386 | 1.00 13.84 | L | 0 |
| | | | | | | | | | | | |
| | MOTA | 1018 | CB | VAL L 133 | | -11.935 | 28.585 104.0 | | 1.00 16.50 | L | C |
| | ATOM | 1019 | CG1 | VAL L 133 | | -10.401 | 28.419 103.7 | 41 | 1.00 12.48 | L | С |
| | ATOM | 1020 | | | • | | 27.202 103.7 | | | | |
| | | | CGZ | VAL L 133 | | -12.729 | | | 1.00 11.93 | L | C |
| | MOTA | 1021 | N | CYS L 134 | | -10.052 | 29.967 106.3 | 318 | 1.00 16.38 | L | N |
| 60 | ATOM | 1022 | CA | CYS L 134 | | -9.164 | | | | | |
| 50 | | | | | | | 31.037 106.6 | | 1.00 17.53 | L | С |
| | ATOM | 1023 | С | CYS L 134 | | -7.833 | 30.655 105.9 | 38 | 1.00 16.58 | L | C |
| | MOTA | 1024 | ō | CYS L 134 | | -7.335 | 29.561 106.2 | | 1.00 14.98 | | |
| | | | | | | | | | | L | 0 |
| | ATOM | 1025 | CB | CYS L 134 | | -8.948 | 31.072 108 <i>.</i> 1 | .08 | 1.00 16.98 | L | C |
| | MOTA | 1026 | SG | CYS L 134 | | -7.928 | 32.442 108.6 | | 1.00 39.38 | L | S |
| ee. | | | | | | | | | | | |
| 65 | MOTA | 1027 | N | PHE L 135 | | -7.314 | 31.512 105.0 | | 1.00 15.50 | L | N |
| | MOTA | 1028 | CA | PHE L 135 | | -5.972 | 31.311 104.4 | 79 | 1.00 15.01 | L | С |
| | | | | | | | | | | | |
| | ATOM | 1029 | C | PHE L 135 | | -5.009 | 32.262 105.2 | | 1.00 17.04 | L | С |
| | ATOM | 1030 | 0 | PHE L 135 | | ~5.343 | 33.413 105.4 | 182 | 1.00 18.37 | L | 0 |
| | ATOM | 1031 | ČВ | PHE L 135 | | -5.953 | 31.730 102.9 | | | | |
| | 771 OIJ | T 0 7 T | CL | רכד ע שייי | | -3.333 | 24.120 TO7.3 | 1 | 1.00 15.31 | L | C |

| | , ATOM | 1032 | CG PHE L 1 | | -6.719 | 30.784 102.083 | 1.00 12.44 | L | _ |
|----|--------------|----------------|----------------------------|------------|-----------------------|----------------------------------|--------------------------|--------|------------|
| | MOTA | $1033 \\ 1034$ | CD1 PHE L 1 CD2 PHE L 1 | | -6.530 -7.604 | 29.429 102.170 31.263 101.147 | 1.00 12.71 1.00 14.37 | L L | |
| | ATOM ATOM | 1034 | CE1 PHE L 1 | | -7.221 | 28.534 101.341 | 1.00 16.73 | L | |
| 5 | ATOM | 1036 | CE2 PHE L 1 | | -8.312 | 30.383 100.294 | | L | |
| - | ATOM | 1037 | | | -8.121 | 29.008 100.399 | | L | |
| | MOTA | 1038 | N LEU L 1 | | -3.795 | 31.794 105.502 | | L L | |
| | ATOM | 1039 1040 | CA LEU L 1 | L36 | -2.784 -1.633 | 32.558 106.211 32.347 105.252 | | L | |
| 10 | ATOM ATOM | 1041 | | L36 L36 | -1.013 | 31.271 105.214 | | ī | |
| 10 | ATOM | 1042 | | 136 | -2.528 | 31.937 107.580 | 1.00 15.90 | L | C |
| | MOTA | 1043 | CG LEU L | | -3.800 | 31.929 108.451 | | L | |
| | MOTA | 1044 | | 136 | -4.513 | 30.583 108.271 | | I. | |
| 4 | MOTA | 1045 | CD2 LEU L | | -3.447 -1.385 | 32.085 109.904 33.363 104.444 | | I I | |
| 15 | ATOM | 1046 1047 | N ASN L CA ASN L | | -0.421 | 33.204 103.397 | | I | |
| • | MOTA ATOM | 1047 | CA ASN L | | 0.894 | 33.961 103.467 | | Ī | |
| | MOTA | 1049 | O ASN L | | 0.972 | 35.032 104.011 | 1.00 24.05 | I | |
| | ATOM | 1050 | CB ASN L | | -1.084 | 33.523 102.061 | | Ī | |
| 20 | MOTA | 1051 | | 137 | -2.092 | 32.423 101.574 | | I I | |
| | MOTA | 1052 | OD1 ASN L : | | -2.866 -2.097 | 32.668 100.681 31.263 102.196 | | I | |
| | ATOM ATOM | 1053 1054 | ND2 ASN L | | 1.932 | 33.348 102.874 | | Ī | |
| | MOTA | 1055 | CA ASN L | | 3.265 | 33.911 102.768 | | I | ı G |
| 25 | MOTA | 1056 | C ASN L | 138 | 3.928 | 34.495 104.025 | | I | |
| | MOTA | 1057 | O ASN L | | 4.332 | 35.646 104.061 | | I | |
| | MOTA | 1058 | CB ASN L | | 3.237 2.971 | 34.913 101.603 34.225 100.280 | | I | |
| | MOTA MOTA | 1059 1060 | CG ASN L OD1 ASN L | | 1.863 | 33.812 100.006 | | Ī | |
| 30 | ATOM | 1061 | ND2 ASN L | | 4.008 | 34.077 99.461 | | I | |
| 00 | ATOM | 1062 | N PHE L | | 4.073 | 33.665 105.062 | | · | - |
| | MOTA | 1063 | CA PHE L | 139 | 4.691 | 34.064 106.294 | | I | |
| | ATOM | 1064 | C PHE L | | 6.009 | 33.355 106.496 | | I | |
| 05 | MOTA | 1065 1066 | O PHE L | 139 | 6.316 3.727 | 32.417 105.788 33.800 107.512 | | I | |
| 35 | ATOM ATOM | 1067 | CG PHE L | | 3.218 | 32.377 107.633 | | Ī | |
| | ATOM | 1068 | CD1 PHE L | | 3.931 | 31.434 108.325 | | I | , C |
| | MOTA | 1069 | CD2 PHE L | 139 | 2.004 | 32.004 107.061 | | I | |
| | MOTA | 1070 | CE1 PHE L | | 3.490 | 30.139 108.459 | | I | |
| 40 | ATOM | 1071 | CE2 PHE L CZ PHE L | | $\frac{1.530}{2.278}$ | 30.697 107.197 29.753 107.894 | | I | |
| | ATOM ATOM | 1072 1073 | CZ PHE L N TYR L | | 6.803 | 33.847 107.430 | | Ī | |
| | MOTA | 1074 | | 140 | 8.085 | 33.240 107.797 | 7 1.00 20.95 | I | r C |
| | ATOM | 1075 | C TYR L | 140 | 8.437 | 33.747 109.186 | _ | I | |
| 45 | MOTA | 1076 | O TYR L | | 8.305 | 34.940 109.476 | | I | |
| | MOTA | 1077 | CB TYR L | | 9.215 10.461 | 33.612 106.810 32.818 107.134 | | I | |
| | MOTA MOTA | 1078 1079 | CG TYR L CD1 TYR L | | 11.314 | 33.233 108.144 | | I | <u>-</u> . |
| | MOTA | 1080 | CD2 TYR L | 140 | 10.719 | 31.607 106.502 | 2 1.00 19.61 | I | r c |
| 50 | MOTA | 1081 | CE1 TYR L | | 12.376 | 32.481 108.53 | | 1 | |
| | MOTA | 1082 | CE2 TYR L | | 11.797 | 30.823 106.903 | | I | |
| | MOTA | 1083 | CZ TYR L | 140 | 12.615 13.684 | 31.290 107.930 30.527 108.384 | 1.00 16.01 1.00 20.60 |]] | |
| | MOTA MOTA | 1084 1085 | OH TYR L N PRO L | | 8.867 | 32.855 110.084 | | | Z N |
| 55 | ATOM | 1086 | CA PRO L | | 9.072 | 31.399 109.97 | | . 1 | r C |
| | MOTA | 1087 | C PRO L | 141 | 7.800 | 30.595 109.882 | | | r C |
| | MOTA | 1088 | O PRO L | | 6.705 | 31.153 109.92 | 3 1.00 22.66 | | . 0 |
| | ATOM | 1089 | CB PRO L | | 9.887 | 31.054 111.22' 32.054 112.19' | | | T C |
| 60 | ATOM | 1090 1091 | CG PRO L CD PRO L | | 9.422 9.306 | 33.344 111.40 | | | r C |
| 60 | ATOM ATOM | 1091 | N LYS L | | 7.957 | 29.281 109.76 | | | L N |
| | ATOM | 1093 | CA LYS L | | 6.803 | 28.390 109.52 | 5 1.00 22.07 | 1 | L C |
| | MOTA | 1094 | C LYS L | 142 | 5.852 | 28.206 110.70 | | | r C |
| | ATOM | 1095 | O LYS L | | 4.730 | 27.743 110.52 | | | r C |
| 65 | ATOM | 1096 | CB LYS L | | 7.291 7.871 | 27.011 109.17 26.341 110.40 | | | r C |
| | ATOM ATOM | 1097 1098 | CG LYS L | 1.42 | 8.364 | 24.905 110.12 | | | r c |
| | ATOM | 1099 | CE LYS L | | 9.132 | 24.425 111.36 | 9 1.00 47.96 |] | r c |
| | ATOM | 1100 | NZ LYS L | | 9.840 | 23.118 111.17 | 5 1.00 68.01 | J | r n |

| ATOM 1102 CA ASP L 143 | | ATOM | 1101 | N | ASP L | 143 | 6.286 | 28.540 | 111.908 | 1.00 | 22.51 | L | N |
|--|-----|------|------|-----|-------|-----|---------|--------|---------|------|-------|---|---|
| ATOM 1104 C ASP L 143 | | | | | | | | | | | | | |
| S | | ATOM | 1103 | С | | 143 | 4.215 | 29.252 | 113.125 | 1.00 | 23.08 | L | |
| ATOM 1106 CG ASP L 143 7.574 27.689 114.178 1.00 27.57 L C ATOM 1107 ASP L 143 8.549 28.452 113.962 1.00 27.57 L C ATOM 1108 OD2 ASP L 143 7.660 26.448 114.240 1.00 35.11 L N ATOM 1109 OD2 ASP L 144 3.885 28.567 113.388 1.00 21.65 L C C ATOM 1110 CA LEE L 1444 1.885 28.567 113.388 1.00 21.65 L C C ATOM 1111 CA LEE L 1444 1.885 28.567 113.388 1.00 21.65 L C C ATOM 1112 CB LEE L 1444 1.485 29.993 111.951 1.00 23.73 L C ATOM 1114 CG LEE L 1444 1.486 29.993 111.951 1.00 23.73 L C ATOM 1115 CG2 LEE L 1444 0.978 28.814 111.995 1.00 20.91 L C ATOM 1116 CG2 LEE L 1444 0.978 28.814 111.199 1.00 21.02 L C ATOM 1117 A ASN L 145 -0.164 29.493 114.744 1.00 23.75 L C ATOM 1117 A ASN L 145 -0.164 29.493 114.744 1.00 23.75 L C ATOM 1118 C ASN L 145 -2.531 29.541 115.032 1.00 28.20 L C ATOM 1120 C ASN L 145 -2.531 29.541 115.032 1.00 28.20 L C ATOM 1122 CG ASN L 145 -2.531 29.541 115.032 1.00 28.20 L C ATOM 1122 CG ASN L 145 -2.231 29.541 115.032 1.00 28.20 L C ATOM 1122 CG ASN L 145 -2.231 29.541 115.032 1.00 28.20 L C ATOM 1122 CG ASN L 145 -2.231 29.541 115.032 1.00 28.20 L C ATOM 1122 CG ASN L 145 -2.231 29.541 115.032 1.00 28.20 L C ATOM 1122 CG ASN L 145 -2.231 29.541 115.032 1.00 28.20 L C ATOM 1125 CG ATOM 1126 CA VALL L 146 -3.293 29.481 114.979 1.00 26.85 L N ATOM 1126 CA VALL L 146 -3.293 29.481 114.979 1.00 26.85 L N ATOM 1126 CA VALL L 146 -3.293 29.481 114.979 1.00 26.85 L N ATOM 1133 CG VALL L 146 -3.293 29.481 114.939 1.00 24.01 L C ATOM 1133 CG VALL L 146 -3.293 29.481 | | ATOM | 1104 | 0 | ASP L | 143 | | 30.472 | 113.035 | | | L | 0 |
| APOM 1107 ODI ASP 1 143 8.549 28.452 113.962 1.00 27.511 L O APOM 1108 ODI ASP L 143 7.660 26.448 114.240 1.00 27.511 L O APOM 1110 O T.LE L 144 3.018 28.659 113.301 1.00 22.13 L N APOM 1111 O T.LE L 144 0.733 28.773 114.084 1.00 22.38 L C APOM 1111 O T.LE L 144 0.733 28.773 114.084 1.00 22.38 L C APOM 1111 O T.LE L 144 0.743 28.773 114.084 1.00 22.38 L C APOM 1115 O T.LE L 144 0.748 29.39 114.084 1.00 22.38 L C APOM 1115 O T.LE L 144 0.456 31.143 111.976 1.00 20.91 L C APOM 1115 OCI T.LE L 144 0.324 31.861 10.617 1.00 23.82 L C APOM 1116 ODI T.LE L 144 0.324 31.861 10.617 1.00 23.82 L C APOM 1117 O ASN L 145 -1.252 28.793 115.442 1.00 29.96 L C APOM 1112 O ASN L 145 -1.252 28.793 115.442 1.00 29.96 L C APOM 1120 O ASN L 145 -2.530 30.760 114.907 1.00 29.90 L C APOM 1122 O ASN L 145 -2.530 30.760 114.907 1.00 29.90 L C APOM 1122 O ASN L 145 -2.530 30.760 114.907 1.00 29.90 L C APOM 1124 APOM 1124 APOM 1124 APOM 124 APOM 125 APOM 125 APOM 125 APOM 126 APOM 126 APOM 127 APOM 127 APOM 128 APOM 129 APOM 120 APOM | 5 | MOTA | | CB | ASP L | 143 | | 28.301 | 114.353 | | | L | |
| AROM 1108 OD2 ASP L 143 7.660 26.448 14.240 1.00 35.11 L O AROM 1109 N ILE L 144 1.855 29.567 113.387 1.00 22.165 L C AROM 1111 O ILE L 144 1.855 29.567 113.387 1.00 22.165 L C AROM 1111 O ILE L 144 0.724 27.530 114.087 1.00 22.39 L C AROM 1112 O ILE L 144 0.724 27.530 114.087 1.00 22.39 L C AROM 1113 O ILE L 144 0.724 27.530 114.087 1.00 25.88 L O O AROM 1115 O ILE L 144 0.456 O AROM 1115 O ILE L 144 0.456 O AROM 1115 O ILE L 144 O AROM 1115 O ILE L 144 O AROM 1115 O ILE L 144 O AROM ILE O AROM ILE O ILE L 144 O AROM ILE O AROM ILE O ILE L 144 O AROM ILE O AROM | | | | | | | | | | | | | |
| APOM | | | | | | | | | | | | | |
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| 15 | | | | | | | | | | | | L | |
| ATOM | 15 | MOTA | 1115 | CG2 | ILE L | 144 | | | | 1.00 | 21.02 | L | C |
| ATOM 1118 CA ASN L 145 -1.252 28.793 115.442 1.00 29.06 L C C ATOM 1120 C ASN L 145 -2.531 29.541 115.032 1.00 28.27 L C C ATOM 1121 CB ASN L 145 -2.530 30.760 114.907 1.00 29.90 L O C ATOM 1122 CG ASN L 145 -1.031 28.854 116.956 1.0 31.88 L C C ATOM 1122 CG ASN L 145 -1.031 28.854 116.956 1.0 31.88 L C C ATOM 1122 ND 1124 ND2 ASN L 145 -1.031 28.854 116.956 1.0 64.13 L O ATOM 1125 N VAL L 146 -2.455 28.192 118.780 1.0 064.13 L O ATOM 1126 CA VAL L 146 -2.455 28.192 114.797 1.00 26.85 L N ATOM 1126 CA VAL L 146 -4.855 29.391 114.379 1.00 24.01 L C ATOM 1127 C VAL L 146 -5.892 28.978 114.379 1.00 24.01 L C ATOM 1128 O VAL L 146 -5.903 27.838 115.829 1.00 25.28 L O ATOM 1120 CB VAL L 146 -5.255 28.862 112.986 1.00 22.10 L C ATOM 1130 CG1 VAL L 146 -5.255 28.862 112.986 1.00 22.10 L C ATOM 1131 CG2 VAL L 146 -6.686 29.332 112.602 1.00 20.92 L C ATOM 1133 CA LYS L 147 -6.713 29.932 115.788 1.00 20.98 L N ATOM 1133 CA LYS L 147 -9.153 31.253 115.542 1.00 23.41 L C ATOM 1134 C LYS L 147 -9.153 31.253 115.542 1.00 23.41 L C ATOM 1136 CB LYS L 147 -9.153 31.253 115.542 1.00 23.41 L C ATOM 1136 CB LYS L 147 -9.153 31.253 115.542 1.00 34.97 L C ATOM 1137 CG LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1137 CG LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1136 CB LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1137 CG LYS L 147 -8.480 30.104 119.09 1.00 34.97 L C ATOM 1136 CB LYS L 147 -8.480 30.104 119.09 1.00 34.97 L C ATOM 1136 CB LYS L 147 -8.480 30.104 119.09 1.00 34.97 L C ATOM 1137 CG LYS L 147 -8.480 30.104 119.09 1.00 34.97 L C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C ATOM 1135 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C ATOM 1136 CB LYS L 147 -8.480 30.104 119.09 1.00 34.97 L C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C C ATOM 1156 CB LYS L 148 -1.148 -1.12.05 CB 1.00 20.29 L C C ATOM 1156 CB LYS L 148 -1.148 -1.12.05 CB 1.00 20.29 | | | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | | |
| ATOM 1120 | | | | | | | | | | | | | |
| ATOM 1121 CB ASN L 145 -1.031 28.854 146.956 1.00 31.88 L C ATOM 1122 CG ASN L 145 -1.901 27.857 117.722 1.00 50.47 L C ATOM 1123 ODI ASN L 145 -2.445 28.192 118.780 1.00 64.13 L O ATOM 1124 ND2 ASN L 145 -2.029 26.627 117.201 1.00 26.85 L N ATOM 1125 N VAL L 146 -3.595 28.796 114.797 1.00 26.85 L N ATOM 1127 C VAL L 146 -3.595 28.796 114.797 1.00 24.01 L C ATOM 1128 O VAL L 146 -5.892 28.978 115.396 1.00 21.85 L C ATOM 1129 CB VAL L 146 -5.892 28.978 115.396 1.00 25.28 L O ATOM 1129 CB VAL L 146 -5.595 28.862 112.986 1.00 22.10 L C ATOM 1131 CG2 VAL L 146 -5.595 28.862 112.986 1.00 20.92 L C ATOM 1131 CG2 VAL L 146 -6.686 29.332 112.602 1.00 20.92 L C ATOM 1133 CA LYS L 147 -6.713 29.932 115.788 1.00 20.98 L N ATOM 1133 CA LYS L 147 -7.780 29.647 116.932 1.00 20.98 L N ATOM 1135 CB LYS L 147 -9.099 30.151 116.083 1.00 20.29 L C ATOM 1135 CB LYS L 147 -9.599 30.151 116.083 1.00 20.29 L C ATOM 1136 CB LYS L 147 -9.593 31.253 115.542 1.00 17.79 L C ATOM 1136 CB LYS L 147 -9.594 30.402 118.034 1.00 20.97 L C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 17.79 L C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C ATOM 1136 CB LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 34.97 L C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 34.97 L C ATOM 1140 CD TRP L 148 -10.139 29.328 116.116 1.00 20.17 L N ATOM 1141 N TRP L 148 -10.139 29.328 116.116 1.00 20.17 L C ATOM 1145 CB TRP L 148 -10.139 29.328 116.116 1.00 20.299 | 20 | | | | | | | | | | | | |
| ATOM 1122 CG ASN L 145 -1.901 27.857 117.722 1.00 50.47 L C ATOM 1123 OD1 ASN L 145 -2.445 28.192 118.780 1.00 64.13 L C ATOM 1125 N VAL L 146 -3.595 28.796 114.797 1.00 26.85 L N ATOM 1126 CA VAL L 146 -3.595 28.796 114.797 1.00 26.85 L N ATOM 1127 C VAL L 146 -5.892 28.978 115.396 1.00 21.85 L C ATOM 1128 O VAL L 146 -5.892 28.978 115.396 1.00 21.85 L C ATOM 1129 CB VAL L 146 -5.893 27.838 115.829 1.00 25.28 L O ATOM 1130 CG1 VAL L 146 -5.893 27.838 115.829 1.00 25.28 L O ATOM 1131 CG2 VAL L 146 -6.686 29.332 112.602 1.00 29.94 L C ATOM 1132 N LYS L 147 -6.713 29.932 115.788 1.00 29.40 L C ATOM 1133 CA LYS L 147 -7.780 29.647 116.732 1.00 23.41 L C ATOM 1134 C LYS L 147 -9.999 30.151 116.083 1.00 20.99 L N ATOM 1136 CB LYS L 147 -9.999 30.151 116.083 1.00 20.29 L C ATOM 1136 CB LYS L 147 -9.999 30.151 116.083 1.00 20.29 L C ATOM 1136 CB LYS L 147 -9.999 30.151 116.083 1.00 20.29 L C ATOM 1136 CB LYS L 147 -9.999 30.151 116.083 1.00 20.29 L C ATOM 1138 CD LYS L 147 -9.8480 30.104 119.109 1.00 34.97 L C ATOM 1138 CD LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1138 CD LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 50.25 L C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 50.25 L C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 50.25 L C ATOM 1140 NZ LYS L 148 -10.139 29.328 16.116 1.00 20.177 L C ATOM 1140 NZ LYS L 148 -10.139 29.328 16.116 1.00 20.217 L C ATOM 1145 CB TRP L 148 -12. | 20 | | | | | | | | | | | | |
| ATOM 1123 ODI ASN L 145 -2.029 26.627 117.201 1.00 46.82 L N | | | | | | | | | | | | | |
| 25 | | | | | | | | | | | | | |
| ATOM | | MOTA | 1124 | ND2 | ASN L | 145 | | 26.627 | 117.201 | 1.00 | 46.82 | L | N |
| ATOM | 25 | ATOM | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | | |
| ATOM 1131 CG2 VAL L 146 | 30 | | | _ | | | | | | | | | |
| ATOM 1132 N LYS L 1476.713 29.932 115.788 1.00 20.98 L N ATOM 1133 CA LYS L 1477.780 29.647 116.732 1.00 23.41 L C C ATOM 1135 CB LYS L 1479.099 30.151 116.083 1.00 20.29 L C C ATOM 1135 CB LYS L 1479.099 30.151 116.083 1.00 20.29 L C C ATOM 1135 CB LYS L 1479.099 30.151 116.083 1.00 19.81 L C ATOM 1135 CB LYS L 1479.504 30.402 118.034 1.00 19.81 L C ATOM 1137 CG LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1138 CD LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C C ATOM 1139 CE LYS L 147 -6.825 30.891 120.876 1.00 50.25 L C C ATOM 1139 CE LYS L 147 -6.825 30.891 120.876 1.00 50.25 L C C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 59.80 L N ATOM 1141 N TRP L 148 -10.139 29.328 116.116 1.00 20.17 L N ATOM 1142 CA TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1143 C TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1144 CB TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1145 CB TRP L 148 -12.122 28.657 114.890 1.00 15.88 L C ATOM 1146 CB TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1146 CB TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1149 NEL TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1149 NEL TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CB2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1151 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CB2 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1151 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1151 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CB2 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1151 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.25 L C ATOM 1151 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.26 L N ATOM 1155 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.29 L C ATOM 1155 CB3 TRP L 148 -11.855 29.085 112.337 1.00 22.89 L N ATOM 1155 CB3 TRP L 148 -12.26 29.35 19.09 18.375 1.00 22.89 L N ATOM 1156 CB3 TRP L 148 -12.26 29.35 19.09 18.375 1.00 22.89 L N ATOM 1156 CB3 TRP L 148 -12.26 29.35 19.09 18.375 1.00 22.02 L C ATOM | 00 | | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | | |
| ATOM | | | | | LYS L | 147 | | | | 1.00 | 23.41 | L | C |
| ATOM 1136 CB LYS L 147 -7.504 30.402 118.034 1.00 19.81 L C ATOM 1137 CG LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1138 CD LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C ATOM 1139 CE LYS L 147 -6.825 30.891 120.876 1.00 59.25 L C ATOM 1140 NZ LYS L 147 -6.825 30.891 120.876 1.00 59.80 L N ATOM 1141 N TRP L 148 -10.139 29.328 116.116 1.00 20.17 L N ATOM 1141 N TRP L 148 -11.445 29.785 115.629 1.00 18.95 L C ATOM 1143 C TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1144 O TRP L 148 -12.325 30.181 116.806 1.00 21.21 L C ATOM 1145 CB TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1146 CG TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1146 CG TRP L 148 -12.122 28.657 114.890 1.00 15.88 L C ATOM 1146 CD TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1147 CD1 TRP L 148 -10.513 27.487 113.208 1.00 16.65 L C ATOM 1149 NE1 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1149 NE1 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1150 CEZ TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1151 CE3 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1151 CE3 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CEZ TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1151 CE3 TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CEZ TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CEZ TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CEZ TRP L 148 -11.855 29.085 112.337 1.00 22.24 L N ATOM 1150 CEZ TRP L 148 -11.855 29.085 112.337 1.00 22.25 L C ATOM 1155 N LYS L 149 -15.431 32.431 115.803 1.00 25.88 L C C ATOM 1155 N LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1155 N LYS L 149 -15.437 33.215 116.623 1.00 22.99 L C ATOM 1155 N LYS L 149 -15.437 33.215 116.623 1.00 22.90 L C ATOM 1150 CEZ LYS L 149 -15.437 33.215 116.623 1.00 22.90 L C ATOM 1150 CEZ LYS L 149 -15.437 33.215 116.623 1.00 22.90 1 L C ATOM 1151 CE LYS L 149 -15.437 33.759 120.883 1.00 25.88 L O ATOM 1160 CE LYS L 149 -15.437 33.759 120.883 1.00 25.88 L O ATOM 1161 CD LYS L 149 -15.4 | | | | С | | | | | | | | | |
| ATOM 1138 CD LYS L 147 -8.480 30.104 119.109 1.00 34.97 L C ATOM 1138 CD LYS L 147 -8.242 31.037 120.294 1.00 50.25 L C ATOM 1139 CE LYS L 147 -6.825 30.891 120.876 1.00 56.37 L C ATOM 1140 NZ LYS L 147 -6.704 31.817 122.085 1.00 59.80 L N ATOM 1141 N TRP L 148 -10.139 29.328 116.116 1.00 20.17 L N ATOM 1141 N TRP L 148 -11.445 29.785 115.629 1.00 18.95 L C ATOM 1143 C TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1144 O TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1145 CB TRP L 148 -12.362 29.785 115.629 1.00 18.95 L C ATOM 1144 O TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1145 CB TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1145 CB TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1145 CB TRP L 148 -12.362 19.559 117.838 1.00 20.59 L O ATOM 1146 CG TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1147 CD1 TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1149 NEI TRP L 148 -10.513 27.487 113.208 1.00 16.655 L C ATOM 1149 NEI TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1150 CE2 TRP L 148 -11.285 29.085 112.337 1.00 22.15 L C ATOM 1151 CE3 TRP L 148 -11.285 29.085 112.337 1.00 22.24 L N ATOM 1151 CE3 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1153 CZ3 TRP L 148 -12.2756 30.111 112.040 1.00 14.25 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 29.29 L C ATOM 1155 C LYS L 149 -13.174 31.215 116.623 1.00 29.29 L C ATOM 1157 C LYS L 149 -13.3675 32.909 118.375 1.00 22.89 L N ATOM 1156 CA LYS L 149 -13.3675 32.909 118.375 1.00 22.89 L N ATOM 1156 CA LYS L 149 -13.3675 32.909 118.375 1.00 22.58 L C ATOM 1164 NZ LYS L 149 -13.3675 32.909 118.375 1.00 25.88 L C ATOM 1166 CG LYS L 149 -13.3675 32.909 118.375 1.00 25.88 L C C ATOM 1166 CG LYS L 149 -13.675 32.909 118.375 1.00 25.88 L C C ATOM 1166 C LYS L 149 -13.663 32.519 118.121 1.00 20.57 L C ATOM 1166 C LYS L 149 -13.863 33.759 120.8375 1.00 25.85 L C ATOM 1166 C LYS L 149 -13. | 35 | | | | | | | | | | | | |
| ATOM 1138 CD LYS L 147 | | | | | | | | | | | | | |
| ATOM 1139 CE LYS L 147 | | | | | | | | | | | | | |
| ATOM | | | | | | | | | | | | | |
| ATOM 1141 N TRP L 148 -10.139 29.328 116.116 1.00 20.17 L N ATOM 1142 CA TRP L 148 -11.445 29.785 115.629 1.00 18.95 L C ATOM 1143 C TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1144 O TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1145 CB TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1145 CB TRP L 148 -12.122 28.657 114.890 1.00 15.88 L C ATOM 1146 CG TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1146 CD2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1148 CD2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1148 CD2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1149 Nel TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1151 CE3 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1151 CZ2 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CZ2 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1155 CZ3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1155 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CA LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1155 CA LYS L 149 -13.174 31.215 116.632 1.00 22.89 L N ATOM 1155 CA LYS L 149 -13.174 31.215 116.632 1.00 22.02 L C ATOM 1158 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1156 CE LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1163 NZ LYS L 149 -13.675 32.909 118.375 1.00 22.02 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CA LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 20.57 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -1 | 40 | | | | | | | | | | | | |
| ATOM 1142 CA TRP L 148 -11.445 29.785 115.629 1.00 18.95 L C ATOM 1143 C TRP L 148 -12.362 30.181 116.806 1.00 21.21 L C ATOM 1144 O TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1145 CB TRP L 148 -12.325 29.559 117.838 1.00 20.59 L O ATOM 1146 CG TRP L 148 -12.322 28.657 114.890 1.00 15.88 L C ATOM 1146 CG TRP L 148 -10.513 27.487 113.208 1.00 16.65 L C ATOM 1148 CD2 TRP L 148 -10.513 27.487 113.208 1.00 16.65 L C ATOM 1148 CD2 TRP L 148 -10.513 27.487 113.208 1.00 16.65 L C ATOM 1149 NE1 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1150 CE2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1151 CE3 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1151 CE3 TRP L 148 -11.087 28.513 111.284 1.00 21.655 L C ATOM 1151 CE3 TRP L 148 -11.087 28.513 111.284 1.00 21.655 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1153 CZ3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1155 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CZ TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CZ TRP L 148 -12.884 31.546 117.655 1.00 21.94 L C ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1156 CA LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1156 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 CB LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C C ATOM 1166 CB LYS L | . • | | | | | | | | | | | | |
| ## ATOM | | | 1142 | CA | TRP L | 148 | -11.445 | 29.785 | 115.629 | 1.00 | 18.95 | L | C |
| ATOM | | MOTA | | C | | | | | | | | | |
| ATOM 1146 CG TRP L 148 -11.490 28.422 113.546 1.00 21.74 L C ATOM 1147 CD1 TRP L 148 -10.513 27.487 113.208 1.00 16.65 L C ATOM 1148 CD2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L ATOM 1149 NE1 TRP L 148 -10.281 27.540 111.832 1.00 22.24 L N 50 ATOM 1150 CE2 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1152 CZ2 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1153 CZ3 TRP L 148 -11.205 28.943 109.950 1.00 24.13 L C ATOM 1153 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 N LYS L 149 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1155 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1158 O LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.577 L C ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.577 L C ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.577 L C ATOM 1166 C TLE L 150 -18.803 31.908 116.995 1.00 19.42 L C ATOM 1166 C TLE L 150 -18.803 32.519 118.121 1.00 20.577 L C ATOM 1166 C TLE L 150 -18.803 32.519 118.121 1.00 20.577 L C ATOM 1167 O ILE L 150 -18.803 31.592 119.232 1.00 22.05 L C ATOM 1167 O ILE L 150 -18.752 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
| ATOM 1148 CD2 TRP L 148 -10.513 27.487 113.208 1.00 16.65 L C ATOM 1148 CD2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1149 NE1 TRP L 148 -10.281 27.540 111.832 1.00 22.24 L N 150 ATOM 1150 CE2 TRP L 148 -10.281 27.540 111.832 1.00 22.24 L N 150 CE2 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1152 CZ2 TRP L 148 -11.205 28.943 109.950 1.00 24.13 L C ATOM 1153 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CH2 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1155 CA LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1155 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1158 O LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1161 CD LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1166 C T LE L 150 -16.534 31.808 116.995 1.00 19.42 L C ATOM 1166 C T LE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C T LE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C T LE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C T LE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1168 CB TLE L 150 -18.527 30.516 116.639 1.00 17.66 L C | 45 | | | _ | | | | | | | | | |
| ATOM 1148 CD2 TRP L 148 -11.855 29.085 112.337 1.00 22.15 L C ATOM 1149 NE1 TRP L 148 -10.281 27.540 111.832 1.00 22.24 L N S ATOM 1150 CE2 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 24.13 L C ATOM 1152 CZ2 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 N LYS L 149 -12.106 29.955 109.676 1.00 19.03 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1159 CB LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 17.66 L C | | | | | | | | | | | | | |
| ATOM 1149 NE1 TRP L 148 -10.281 27.540 111.832 1.00 22.24 L N ATOM 1150 CE2 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L ATOM 1152 CZ2 TRP L 148 -11.205 28.943 109.950 1.00 24.13 L C ATOM 1153 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1154 CH2 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.427 31.917 116.932 1.00 22.50 L C ATOM 1150 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1165 CA ILE L 150 -16.534 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -16.534 31.808 116.995 1.00 19.42 L C ATOM 1167 O ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 CB ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 CB ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C | | | | | | | | | | | | | _ |
| 50 ATOM 1150 CE2 TRP L 148 -11.087 28.513 111.284 1.00 21.65 L C ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1152 CZ2 TRP L 148 -11.205 28.943 109.950 1.00 24.13 L C ATOM 1153 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1154 CH2 TRP L 148 -12.106 29.955 109.676 1.00 19.03 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1150 CB LYS L 149 -13.675 32.909 118.375 1.00 25.88 L O ATOM 1160 CG LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N TLE L 150 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N TLE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O TLE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1168 CB TLE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB TLE L 150 -18.735 31.982 119.232 1.00 20.57 L C | | | | | | | | | | | | | |
| ATOM 1151 CE3 TRP L 148 -12.756 30.111 112.040 1.00 14.25 L C ATOM 1152 CZ2 TRP L 148 -11.205 28.943 109.950 1.00 24.13 L C ATOM 1153 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1155 N LYS L 149 -12.106 29.955 109.676 1.00 19.03 L C 55 ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1159 CB LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1160 CG LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C TLE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C TLE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1166 C TLE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L | 50 | ATOM | | | | | | | | | | | |
| ATOM 1153 CZ3 TRP L 148 -12.884 30.542 110.716 1.00 20.29 L C ATOM 1154 CH2 TRP L 148 -12.106 29.955 109.676 1.00 19.03 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.427 31.917 116.932 1.00 22.50 L C ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1165 CA ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N ATOM 1166 C ILE L 150 -16.534 31.563 117.575 1.00 22.57 L C ATOM 1166 C ILE L 150 -18.735 31.982 119.232 1.00 22.05 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O | | | | CE3 | | | | | | | | | C |
| ATOM 1154 CH2 TRP L 148 -12.106 29.955 109.676 1.00 19.03 L C ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L | | | | | | | | | | | | | |
| 55 ATOM 1155 N LYS L 149 -13.174 31.215 116.623 1.00 22.89 L N ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 66 ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L | | | | | | | | | | | | | |
| ATOM 1156 CA LYS L 149 -14.124 31.636 117.655 1.00 21.94 L C ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 66 ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L | | | | | | | | | | | | | |
| ATOM 1157 C LYS L 149 -15.427 31.917 116.932 1.00 22.02 L C ATOM 1158 O LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1168 CB ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L | 55 | | | | | | | | | | | | |
| ATOM 1158 O LYS L 149 -15.431 32.431 115.803 1.00 25.88 L O ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1161 CD LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1162 CE LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1163 NZ LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1164 N ILE L 150 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1166 C ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
| ATOM 1159 CB LYS L 149 -13.675 32.909 118.375 1.00 22.50 L C ATOM 1160 CG LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
| 60 ATOM 1160 CG LYS L 149 -12.456 32.712 119.265 1.00 29.41 L C ATOM 1161 CD LYS L 149 -11.972 34.038 119.890 1.00 36.17 L C ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
| ATOM 1162 CE LYS L 149 -10.853 33.759 120.883 1.00 47.79 L C ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | 60 | | | CG | | | -12.456 | | | 1.00 | 29.41 | L | C |
| ATOM 1163 NZ LYS L 149 -10.191 35.022 121.349 1.00 58.02 L N ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | CD | LYS L | 149 | | | | | | L | C |
| ATOM 1164 N ILE L 150 -16.534 31.563 117.575 1.00 21.85 L N 65 ATOM 1165 CA ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
| 65 ATOM 1165 CA ILE L 150 -17.842 31.808 116.995 1.00 19.42 L C ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
| ATOM 1166 C ILE L 150 -18.603 32.519 118.121 1.00 20.57 L C ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | 65 | | | | | | | | | | | | |
| ATOM 1167 O ILE L 150 -18.735 31.982 119.232 1.00 22.05 L O ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | 00 | | | | | | | | | | | | |
| ATOM 1168 CB ILE L 150 -18.527 30.516 116.639 1.00 17.66 L C | | | | | | | | | | | | | |
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| | 14 ······· 14 | | | | | | | |
|----|-----------------|------|---------------|---------|----------------|------------|------------------|------------|
| | ATOM | 1170 | CG2 ILE L 150 | -20.013 | 30.809 116.281 | 1.00 15.45 | L | С |
| | | 1171 | CD1 ILE L 150 | -18,484 | 28.535 114.955 | 1.00 5.50 | L | Č |
| | ATOM | | | | 33.734 117.831 | 1.00 20.49 | Ŀ | N |
| | MOTA | 1172 | N ASP L 151 | -19.030 | | | | |
| | ATOM | 1173 | CA ASP L 151 | -19.715 | 34.559 118.815 | 1.00 20.94 | L | C |
| 5 | MOTA | 1174 | C ASP L 151 | -18.815 | 34.701 120.052 | 1.00 24.12 | L | С |
| _ | ATOM | 1175 | O ASP L 151 | -19.304 | 34.789 121.189 | 1.00 24.25 | L | 0 |
| | | 1176 | CB ASP L 151 | -21.059 | 33.894 119.175 | 1.00 19.59 | L | С |
| | ATOM | | | | 34.129 118.102 | 1.00 25.62 | Ŀ | č |
| | ATOM | 1177 | CG ASP L 151 | -22.132 | 34.129 110.102 | | | |
| | MOTA | 1178 | OD1 ASP L 151 | -21.968 | 35.055 117.272 | 1.00 27.32 | L | 0 |
| 10 | MOTA | 1179 | OD2 ASP L 151 | -23.152 | 33.416 118.110 | 1.00 31.24 | L | 0 |
| | ATOM | 1180 | N GLY L 152 | -17.493 | 34.685 119.850 | 1.00 19.02 | L | N |
| | ATOM | 1181 | CA GLY L 152 | -16.617 | 34.845 120.990 | 1.00 23.51 | L | С |
| | | | | -16.141 | 33.602 121.724 | 1.00 28.41 | | Ċ |
| | ATOM | 1182 | C GLY L 152 | | | | | |
| | MOTA | 1183 | O GLY L 152 | -15.242 | 33.688 122.577 | 1.00 32.84 | L | 0 |
| 15 | ATOM | 1184 | N SER L 153 | -16.732 | 32.458 121.438 | 1.00 28.85 | L | N |
| | ATOM | 1185 | CA SER L 153 | -16.307 | 31.209 122.065 | 1.00 29.03 | L | С |
| | ATOM | 1186 | C SER L 153 | -15.417 | 30.391 121.122 | 1.00 28.97 | L | C |
| | | | | -15.757 | 30.161 119.960 | 1.00 26.39 | L | O |
| | MOTA | 1187 | | | | 1.00 25.23 | L | č |
| | ATOM | 1188 | CB SER L 153 | -17.505 | 30.360 122.471 | | | |
| 20 | MOTA | 1189 | OG SER L 153 | -18.196 | 31.006 123.519 | 1.00 30.72 | L | 0 |
| | MOTA | 1190 | N GLU L 154 | -14.283 | 29.942 121.643 | 1.00 28.12 | L | N |
| | ATOM | 1191 | CA GLU L 154 | -13.380 | 29.141 120.842 | 1.00 31.33 | L | C |
| | MOTA | 1192 | C GLU L 154 | -14.031 | 27.826 120.432 | 1.00 31.48 | L | С |
| | | | | -14.753 | 27.175 121.200 | 1.00 35.29 | Ŀ | ō |
| | MOTA | 1193 | O GLU L 154 | | | | | |
| 25 | MOTA | 1194 | CB GLU L 154 | -12.091 | 28.879 121.635 | 1.00 32.78 | | C |
| | ATOM | 1195 | CG GLU L 154 | -11.053 | 28.084 120.877 | 1.00 40.84 | L | C |
| | MOTA | 1196 | CD GLU L 154 | -9.769 | 27.927 121.683 | 1.00 43.42 | L | С |
| | MOTA | 1197 | OE1 GLU L 154 | -9.576 | 28.679 122.656 | 1.00 47.11 | L | 0 |
| | | 1198 | OE2 GLU L 154 | -8.966 | 27.061 121.335 | 1.00 52.41 | L | 0 |
| | ATOM | | | | | 1.00 28.45 | Ŀ | N |
| 30 | ATOM | 1199 | N ARG L 155 | -13.793 | 27.435 119.196 | | | |
| | MOTA | 1200 | CA ARG L 155 | -14.309 | 26.189 118.675 | 1.00 30.91 | L | C |
| | MOTA | 1201 | C ARG L 155 | -13.115 | 25.406 118.252 | 1.00 32.16 | L | - C |
| | ATOM | 1202 | O ARG L 155 | -12.374 | 25.876 117.405 | 1.00 32.66 | L | 0 |
| | MOTA | 1203 | CB ARG L 155 | -15.183 | 26.419 117.448 | 1.00 28.52 | L | C |
| 0- | | | CD ANG D 155 | | 27.231 117.799 | 1.00 37.92 | L | Č |
| 35 | MOTA | 1204 | CG ARG L 155 | -16.380 | | | | |
| | MOTA | 1205 | CD ARG L 155 | -17.336 | 26.438 118.698 | 1.00 31.38 | L | C |
| | MOTA | 1206 | NE ARG L 155 | -18.612 | 27.118 118.747 | 1.00 33.65 | L | . N |
| | MOTA | 1207 | CZ ARG L 155 | -19.691 | 26.762 118.062 | 1.00 17.41 | \mathbf{L}_{t} | С |
| | MOTA | 1208 | NH1 ARG L 155 | -19.685 | 25.711 117.260 | 1.00 27.68 | L | N |
| 40 | | | NH2 ARG L 155 | -20.780 | 27.482 118.185 | 1.00 25.10 | L | N |
| 40 | ATOM | 1209 | * | | | 1.00 34.52 | Ĺ | N |
| | MOTA | 1210 | N GLN L 156 | -12.935 | 24.221 118.829 | | | |
| | MOTA | 1211 | CA GLN L 156 | -11.788 | 23.395 118.478 | 1.00 35.80 | L | C |
| | ATOM | 1212 | C GLN L 156 | -12.127 | 22.210 117.605 | 1.00 36.43 | L | С |
| | ATOM | 1213 | O GLN L 156 | -11.293 | 21.749 116.805 | 1.00 39.56 | L | 0 |
| 45 | ATOM | 1214 | CB GLN L 156 | -11.078 | 22.906 119.743 | 1.00 33.20 | L | С |
| 40 | | 1215 | CG GLN L 156 | | 24.010 120.664 | 1.00 47.03 | L | С |
| | MOTA | | | | | 1.00 57.66 | Ľ | č |
| | MOTA | 1216 | CD GLN L 156 | | | | | - |
| | ATOM | 1217 | OE1 GLN L 156 | ~10.360 | 22.685 122.634 | 1.00 72.71 | Ē | 0 |
| | MOTA | 1218 | NE2 GLN L 156 | -8.643 | 23.981 121.977 | 1.00 63.16 | L | N |
| 50 | MOTA | 1219 | N ASN L 157 | | 21.698 117.723 | 1.00 38.17 | L | N |
| | ATOM | 1220 | CA ASN L 157 | | | 1.00 38.15 | L | С |
| | | | | -14.121 | | 1.00 35.01 | L | C |
| | ATOM | 1221 | C ASN L 157 | -14.121 | 20.000 115.374 | 1.00 34.08 | Ĺ | Õ |
| | \mathtt{MOTA} | 1222 | O ASN L 157 | | | | | |
| | MOTA | 1223 | CB ASN L 157 | | | 1.00 43.26 | L | Ç |
| 55 | MOTA | 1224 | CG ASN L 157 | ~14.457 | 19.007 118.785 | 1.00 57.31 | L | C |
| | MOTA | 1225 | OD1 ASN L 157 | -15.297 | | 1.00 74.40 | L | 0 |
| | | | ND2 ASN L 157 | | | 1.00 54.46 | L | N |
| | ATOM | 1226 | NDZ ASN L 157 | 12.007 | | 1.00 32.01 | Ŀ | N |
| | MOTA | 1227 | N GLY L 158 | | | | | |
| | MOTA | 1228 | CA GLY L 158 | | | 1.00 26.62 | Ŀ | C |
| 60 | MOTA | 1229 | C GLY L 158 | -13.389 | 21.035 112.359 | 1.00 26.13 | L | C |
| - | ATOM | 1230 | O GLY L 158 | | | 1.00 26.96 | L | 0 |
| | | 1231 | N VAL L 159 | | | 1.00 22.23 | L | N |
| | MOTA | | | | | 1.00 23.71 | L | Ĉ |
| | MOTA | 1232 | CA VAL L 159 | | | | | |
| | MOTA | 1233 | C VAL L 159 | | | 1.00 25.37 | L | G |
| 65 | MOTA | 1234 | O VAL L 159 | | | 1.00 34.95 | L | 0 |
| | ATOM | 1235 | CB VAL L 159 | -10.376 | 22.820 113.140 | 1.00 19.67 | ь | C |
| | MOTA | 1236 | CG1 VAL L 159 | | | 1.00 26.30 | L | C |
| | MOTA | 1237 | CG2 VAL L 159 | | | 1.00 16.36 | L | C |
| | | | | | | 1.00 29.08 | L | Ŋ |
| | MOTA | 1238 | N LEU L 160 | -9.094 | 77.401 TIO.012 | 1.00 49.00 | اساد | 7./ |

| | ATOM | 1239 | CA LEU L 160 | -8.948 | 20.728 109.219 | 1.00 29.44 1.00 24.79 | L | C C |
|----|--------------|---------------------|------------------------------|------------------|----------------------------------|--------------------------|--------------|----------|
| | MOTA | 1240 | C LEU L 160 | -7.885 | 21.763 108.832 | 1.00 24.79 1.00 25.27 | L L | 0 |
| | ATOM | 1241 | O LEU L 160 | -8.238 | 22.824 108.320 20.233 107.946 | 1.00 25.27 | r L | C |
| - | ATOM | 1242 | CB LEU L 160 CG LEU L 160 | -9.658 -8.866 | 19.400 106.916 | 1.00 23.33 | Ŀ | Č |
| 5 | MOTA | $\frac{1243}{1244}$ | CG LEU L 160 | -9.801 | 18.461 106.149 | 1.00 38.99 | Ŀ | č |
| | MOTA MOTA | 1245 | CD2 LEU L 160 | -8.126 | 20.321 105.949 | 1.00 53.32 | Ĺ | Č |
| | ATOM | 1245 | N ASN L 161 | -6.625 | 21.455 109.089 | 1.00 21.11 | L | N |
| | MOTA | 1247 | CA ASN L 161 | -5.543 | 22.387 108.800 | 1.00 19.49 | L | C |
| 10 | ATOM | 1248 | C ASN L 161 | -4,602 | 21.752 107.801 | 1.00 18.69 | L | C |
| 10 | ATOM | 1249 | O ASN L 161 | -4.409 | 20.538 107.838 | 1.00 21.55 | L | 0 |
| | ATOM | 1250 | CB ASN L 161 | -4.759 | 22.717 110.086 | 1.00 19.31 | L | C |
| | ATOM | 1251 | CG ASN L 161 | -5.511 | 23.651 111.029 | 1.00 12.67 | L | C |
| | ATOM | 1252 | OD1 ASN L 161 | -6.298 | 24.476 110.607 | 1.00 21.51 | L | 0 |
| 15 | ATOM | 1253 | ND2 ASN L 161 | -5.232 | 23.539 112.311 | 1.00 27.96 | · L | N |
| | MOTA | 1254 | N SER L 162 | -4.045 | 22.557 106.886 | 1.00 17.66 | L | N |
| | ATOM | 1255 | CA SER L 162 | -3.099 | 22.029 105.898 | 1.00 20.32 | Ē | C |
| | MOTA | 1256 | C SER L 162 | -2.031 | 23.129 105.737 | 1.00 20.31 | Ŀ | C |
| | ATOM | 1257 | O SER L 162 | -2.347 | 24.344 105.761 | 1.00 20.48 | L | 0 |
| 20 | MOTA | 1258 | CB SER L 162 | -3.766 | 21.771 104.569 21.096 103.721 | 1.00 19.36 1.00 30.64 | L L | C O |
| | MOTA | 1259 | OG SER L 162 | -2.842 -0.776 | 22.711 105.539 | 1.00 30.64 | L | И |
| | ATOM | 1260 1261 | N TRP L 163 CA TRP L 163 | 0.320 | 23.662 105.444 | 1.00 22.30 | L | C |
| | MOTA MOTA | 1262 | C TRP L 163 | 1.127 | 23.380 104.181 | 1.00 16.75 | Ĺ | Č |
| 25 | ATOM | 1263 | O TRP L 163 | 1.325 | 22.217 103.821 | 1.00 20.55 | L | ō |
| 20 | ATOM | 1264 | CB TRP L 163 | 1.231 | 23.485 106.662 | 1.00 13.33 | L | C |
| | ATOM | 1265 | CG TRP L 163 | 0.544 | 23.657 108.029 | 1.00 22.80 | L | C |
| | MOTA | 1266 | CD1 TRP L 163 | 0.495 | 24.786 108.763 | 1.00 19.32 | L | С |
| | ATOM | 1267 | CD2 TRP L 163 | -0.167 | 22.651 108.791 | 1.00 26.71 | L | С |
| 30 | ATOM | 1268 | NE1 TRP L 163 | -0.199 | 24.560 109.945 | 1.00 30.77 | L | N |
| | MOTA | 1269 | CE2 TRP L 163 | -0.614 | 23.259 109.977 | 1.00 26.86 | L | C |
| | MOTA | 1270 | CE3 TRP L 163 | -0.463 | 21.302 108.575 | 1.00 32.13 | Ļ | C |
| | MOTA | 1271 | CZ2 TRP L 163 | -1.350 | 22.569 110.961 | 1.00 26.97 | Ļ | C |
| | MOTA | 1272 | CZ3 TRP L 163 | -1.199 | 20.595 109.565 | 1.00 31.68 | L L | C |
| 35 | ATOM | 1273 | CH2 TRP L 163 | -1.629 | 21.243 110.738 | 1.00 37.55 | P P | N |
| | MOTA | 1274 | N THR L 164 | 1.600 | 24.416 103.506 24.192 102.285 | 1.00 19.49 1.00 18.40 | Г Г | C |
| | MOTA | 1275 | CA THR L 164 C THR L 164 | 2.412 3.871 | 24.192 102.283 | 1.00 18.40 | L | Č |
| | MOTA | 1276 1277 | C THR L 164 O THR L 164 | 4.263 | 24.324 103.801 | 1.00 18.48 | Ŀ | ŏ |
| 40 | MOTA MOTA | 1278 | CB THR L 164 | 2.367 | 25.378 101.286 | 1.00 16.10 | L | Č |
| 40 | ATOM | 1279 | OG1 THR L 164 | 2.767 | 26.598 101.961 | 1.00 22.69 | _ L | ō |
| | ATOM | 1280 | CG2 THR L 164 | 0.978 | 25.562 100.694 | 1.00 20.82 | L | C |
| | MOTA | 1281 | N ASP L 165 | 4.664 | 23.505 101.739 | 1.00 22.96 | L | N |
| | ATOM | 1282 | CA ASP L 165 | 6.095 | 23.397 101.939 | 1.00 23.19 | \mathbf{L} | C |
| 45 | MOTA | 1283 | C ASP L 165 | 6.590 | 24.820 101.584 | 1.00 18.88 | L | C |
| | MOTA | 1284 | O ASP L 165 | 5.850 | 25.633 101.007 | 1.00 18.60 | L | 0 |
| | MOTA | 1285 | CB ASP L 165 | 6.699 | 22.432 100.915 | 1.00 30.01 | Ŀ | Č |
| | MOTA | 1286 | CG ASP L 165 | 6.309 | 20.986 101.155 | 1.00 40.64 | Ļ | C |
| | MOTA | 1287 | OD1 ASP L 165 | 5.882 | 20.384 100.158 | 1.00 52.97 | L | 0 |
| 50 | MOTA | 1288 | OD2 ASP L 165 | 6.452 | 20.460 102.298 | 1.00 38.53 1.00 13.81 | r r | N O |
| | ATOM | 1289 | N GLN L 166 | 7.848 8.415 | 25.089 101.885 26.424 101.625 | 1.00 13.81 | Ľ | C |
| | MOTA | 1290 | CA GLN L 166 C GLN L 166 | 8.333 | 26.806 100.156 | 1.00 12.21 | Ľ | C |
| | MOTA MOTA | 1291 1292 | C GLN L 166 O GLN L 166 | 8.604 | 26.014 99.290 | 1.00 16.65 | Ŀ | õ |
| 55 | ATOM | 1293 | CB GLN L 166 | 9.845 | 26.458 102.164 | 1.00 12.35 | L L | č |
| 55 | MOTA | 1294 | CG GLN L 166 | 10.442 | 27.875 102.139 | 1.00 12.75 | L | C |
| | MOTA | 1295 | CD GLN L 166 | 11.704 | 27.936 102.959 | 1.00 16.64 | L | С |
| | MOTA | 1296 | OE1 GLN L 166 | 12.504 | 26.974 102.995 | 1.00 22.95 | L | 0 |
| | ATOM | 1297 | NE2 GLN L 166 | 11.900 | 29.050 103.628 | 1.00 15.16 | L | N |
| 60 | MOTA | 1298 | N ASP L 167 | 7.920 | 28.036 99.874 | 1.00 15.54 | L | N |
| | MOTA | 1299 | CA ASP L 167 | 7.768 | 28.520 98.523 | 1.00 17.06 | L | С |
| | ATOM | 1300 | C ASP L 167 | 9.168 | 28.649 97.864 | 1.00 17.69 | Ŀ | C |
| | ATOM | 1301 | O ASP L 167 | 10.151 | 29.093 98.482 | 1.00 17.79 | Ŀ | 0 |
| | MOTA | 1302 | CB ASP L 167 | 7.095 | 29.908 98.508 | 1.00 13.53 | L | C |
| 65 | MOTA | 1303 | CG ASP L 167 | 6.785 | 30.356 97.119 | 1.00 22.46 | L | C |
| | ATOM | 1304 | OD1 ASP L 167 | 5.750 | 29.917 96.602 | 1.00 24.43 | L | 0 |
| | MOTA | 1305 | OD2 ASP L 167 | 7.597 | 31.127 96.514 | 1.00 25.80 1.00 21.93 | L L | N O |
| | MOTA | 1306 | N SER L 168 | 9.191 10.385 | 28.257 96.607 28.290 95.761 | 1.00 21.93 | r L | G 1/4 |
| | ATOM | 1307 | CA SER L 168 | 10.363 | 40.290 33.10I | I | 11 | • |

| | | | | | | | | | | _ | |
|----|--------------|--------------|---------|----------------|-----|------------------|------------------|--------------------|--------------------------|-----|-----|
| | ATOM | 1308 | C | SER L | | 10.858 | 29.659 | 95.322 | 1.00 23.47 | | C |
| | MOTA | 1309 | 0 | | 168 | 11.999 | 29.782 | 94.879 | 1.00 25.30 | | |
| | ATOM | 1310 | CB | SER L | | 10.133 | 27.465 | 94.480 | 1.00 17.84 | | |
| _ | ATOM | 1311 | OG | SER L | | 10.011 | 26.117 | 94.892 | 1.00 38.05 | | |
| 5 | MOTA | 1312 | N | LYS L | | 10.005 10.397 | 30.657 31.989 | 95.398 94.958 | 1.00 20.43 | | |
| | ATOM | 1313 | CA | LYS L | | 10.337 | 32.922 | 96.114 | 1.00 20.10 | | |
| | ATOM ATOM | 1314 1315 | C C | LYS L | | 11.610 | 33.623 | 96.145 | 1.00 19.99 | | |
| | ATOM | 1316 | CB | LYS L | | 9.319 | 32.574 | 94.021 | 1.00 21.29 | | |
| 10 | MOTA | 1317 | CG | LYS L | | 9.239 | 31.821 | 92.667 | 1.00 30.1 | | |
| 10 | ATOM | 1318 | CD | LYS L | | 8.116 | 32.333 | 91.773 | 1.00 44.03 | | |
| | MOTA | 1319 | CE | LYS L | | 8.244 | 31.763 | 90.356 | 1.00 57.38 | 3 ь | C |
| | ATOM | 1320 | NZ | LYS L | | 7.258 | 32.403 | 89.414 | 1.00 70.7 | | |
| | MOTA | 1321 | N | ASP L | 170 | 9.699 | 32.972 | 97.083 | 1.00 23.10 | | |
| 15 | ATOM | 1322 | CA | ASP L | | 9.915 | 33.914 | 98.176 | 1.00 20.43 | | |
| | MOTA | 1323 | C | ASP L | | 10.240 | 33.309 | 99.528 | 1.00 22.49 | | |
| | MOTA | 1324 | 0 | ASP L | | 10.345 | 34.018 | | 1.00 24.0 | | |
| | MOTA | 1325 | CB | ASP L | | 8.719 | 34.874 | 98.269 | 1.00 23.5 | | |
| | MOTA | 1326 | CG | ASP L | | 7.420 | 34.180 | 98.769 | 1.00 28.5 | | |
| 20 | ATOM | 1327 | | ASP L | | 7.457 6.362 | 33.006 34.859 | 99.213 98.753 | 1.00 28.25 1.00 32.05 | | |
| | MOTA | 1328 | | ASP L SER L | | 10.437 | 31.980 | 99.555 | 1.00 32.0 | | |
| | MOTA ATOM | 1329 1330 | N CA | SER L | | 10.854 | 31.272 | | 1.00 19.5 | | |
| | MOTA | 1331 | C | SER L | 171 | 9.905 | 31.416 | | 1.00 18.9 | | |
| 25 | MOTA | 1332 | ŏ | SER L | | 10.332 | 31.277 | | 1.00 20.8 | | |
| 20 | ATOM | 1333 | СB | SER L | | 12.260 | | 101.193 | 1.00 16.8 | | |
| | MOTA | 1334 | ŌĠ | SER L | | 13.092 | 31.639 | 100.049 | 1.00 22.6 | 4 L | 0 |
| | MOTA | 1335 | N | THR L | | 8.629 | 31.627 | 101.661 | 1.00 17.1 | | |
| | ATOM | 1336 | CA | THR L | 172 | 7.634 | | 102.747 | 1.00 17.2 | | |
| 30 | MOTA | 1337 | C | THR L | | 6.824 | | 102.837 | 1.00 15.1 | | |
| | ATOM | 1338 | 0 | THR L | 172 | 6.950 | | 101.988 | 1.00 13.2 | | |
| | MOTA | 1339 | СВ | THR L | | 6.619 | | 102.488 | 1.00 15.9 | | |
| | ATOM | 1340 | | THR L | | 5.904 | | 101.251 | 1.00 24.2 | | |
| | MOTA | 1341 | CG2 | | | 7.382 | | 102.381 | 1.00 10.4 | | |
| 35 | MOTA | 1342 | N | TYR L | | 5.959 | | 103.849 104.100 | 1.00 14.8 1.00 13.9 | | |
| | MOTA | 1343 | CA | TYR L | | 5.091 3.666 | | 104.100 | 1.00 15.9 | | |
| | ATOM ATOM | 1344 1345 | C. | TYR L | | 3.442 | 31.018 | | 1.00 11.8 | | |
| | ATOM | 1345 | CB | TYR L | | 5.366 | | 105.488 | 1.00 12.0 | | |
| 40 | ATOM | 1347 | CG | TYR L | | 6.732 | 28.076 | | 1.00 19.9 | | |
| 40 | ATOM | 1348 | CD1 | | | 7.827 | 28.832 | | 1.00 18.4 | _ | |
| | ATOM | 1349 | CD2 | | | 6.937 | 26.749 | | 1.00 12.6 | 3 L | |
| | MOTA | 1350 | CE1 | | | 9.092 | | 106.067 | 1.00 28.5 | | |
| | ATOM | 1351 | CE2 | | | 8.216 | | 105.287 | 1.00 20.2 | | |
| 45 | MOTA | 1352 | CZ | TYR L | | 9.276 | | 105.713 | 1.00 20.8 | | |
| | MOTA | 1353 | OH | TYR L | | 10.530 | | 105.841 | 1.00 31.8 | | |
| | ATOM | 1354 | N | | | 2.706 | 28.892 | 103.891 | 1.00 17.0 | 8 L | N |
| | ATOM | 1355 | CA | SER L | | 1.281 | | 103.906 | 1.00 14.7 1.00 15.2 | | |
| 50 | MOTA | 1356 | C | SER L | | 0.465 0.924 | | 104.737 | 1.00 13.2 | | |
| 50 | ATOM ATOM | 1357 1358 | O CB | SER L | | 0.770 | | 102.491 | 1.00 16.5 | | |
| | ATOM | 1359 | OG | SER L | | 1.300 | | 101.906 | 1.00 16.1 | | |
| | MOTA | 1360 | N | MET L | | -0.753 | | 105.046 | 1.00 16.1 | | |
| | ATOM | 1361 | CA | MET L | | -1.562 | | 105.762 | 1.00 13.0 | 1 I | |
| 55 | ATOM | 1362 | C | MET L | | -3.020 | | 105.431 | 1.00 14.5 | | , C |
| | MOTA | 1363 | 0 | MET L | | -3.417 | 28.949 | 105.198 | 1.00 17.5 | | |
| | MOTA | 1364 | CB | MET L | | -1.381 | | 107.296 | 1.00 13.6 | | |
| | ATOM | 1365 | CG | MET L | | -2.422 | | 108.210 | 1.00 11.5 | | |
| | ATOM | 1366 | SD | MET L | | -2.089 | | 109.942 | 1.00 19.8 | | |
| 60 | MOTA | 1367 | CE | MET L | | -3.279 | | 110.822 | 1.00 19.3 | | |
| | MOTA | 1368 | N | SER L | | -3.803 | | 105.418 | 1.00 12.1 | | |
| | ATOM | 1369 | CA | SER I | | -5.268 | | 105.196 | 1.00 12.4 | | |
| | ATOM | 1370 | C | SER L | | -5.934 5.486 | | 106.436 | 1.00 14.5 1.00 13.6 | | |
| 65 | MOTA | 1371 | 0 | SER L | | -5.486 -5.673 | | 108.909 | 1.00 13.6 | | |
| 65 | MOTA | 1372 1373 | CB | SER I SER I | | -5.673 -7.084 | | 103.962 | 1.00 16.8 | | |
| | MOTA MOTA | 1374 | OG N | SER L | | -6.986 | | 106.972 | 1.00 14.3 | | |
| | ATOM | 1375 | CA | SER I | | -7.641 | | 108.128 | 1.00 14.3 | | |
| | ATOM | 1376 | C | SER I | | -9.113 | | 107.753 | 1.00 16.2 | | |
| | | | | | | | | | | | |

| | | | | | | | | | | | | _ |
|-----|-----------|--------------------|-------------|---------|-----|---------|--------|---------|------|-------|----------|---|
| | ATOM | 1377 | 0 | SER L | 177 | -9.583 | | 107.371 | | 19.72 | Ŀ | 0 |
| | MOTA | 1378 | CB | SER L | 177 | -7.412 | 26.992 | 109.379 | 1.00 | 10.63 | Ŀ | C |
| | MOTA | 1379 | OG | SER L | 177 | -7.994 | 26.377 | 110.518 | 1.00 | 18.28 | <u> </u> | 0 |
| | ATOM | 1380 | N | THR L | 178 | -9.823 | 25.089 | 107.862 | 1.00 | 18.72 | L) | N |
| 5 | ATOM | 1381 | CA | THR L | 178 | -11.227 | 25.063 | 107.512 | 1.00 | 19.80 | L L | C |
| • | ATOM | 1382 | C | THR L | | -12.029 | 24.577 | 108.721 | | 19.45 | L | C |
| | ATOM | 1383 | ŏ | THR L | | -11.728 | | 109.262 | | 19.44 | L | 0 |
| | ATOM | 1384 | ČВ | THR L | | -11.483 | | 106.371 | | 17.81 | _ L | C |
| | ATOM | 1385 | OG1 | | | -10.737 | | 105.195 | | 20.86 | _ L | Õ |
| 10 | | 1386 | CG2 | THR L | | -12.952 | | 106.014 | | 20.63 | L L | č |
| 10 | MOTA | | | LEU L | | -13.001 | | 100.014 | | 16.56 | L | Й |
| | MOTA | 1387 1388 | N | LEU L | | -13.874 | | 110.279 | | 19.50 | L | C |
| | ATOM | | CA | | | | | | | 19.78 | L L | C |
| | MOTA | 1389 | Ğ | LEU L | | -15.197 | | 109.628 | | 19.78 | | |
| | MOTA | 1390 | 0_ | LEU L | | -15.884 | | 108.957 | | | L | 0 |
| 15 | ATOM | 1391 | CB | LEU L | | -14.157 | | 111.207 | | 18.74 | <u></u> | C |
| | MOTA | 1392 | CG | LEU L | | -15.233 | | 112.315 | | 19.17 | L | C |
| | MOTA | 1393 | | LEU L | | -14.778 | | 113.287 | | 22.85 | L - | C |
| | MOTA | 1394 | CD2 | LEU L | | -15.411 | | 113.049 | | 13.61 | L | С |
| | ATOM | 1395 | N | THR L | | -15.558 | | 109.836 | | 16.39 | L | N |
| 20 | MOTA | 1396 | $^{\rm CA}$ | THR L | 180 | -16.778 | | 109.226 | | 22.47 | L | С |
| | MOTA | 1397 | С | THR L | 180 | -17.911 | 22.551 | 110.243 | | 22.40 | L | С |
| | ATOM | 1398 | 0 | THR L | 180 | -17.733 | 22.007 | 111.335 | 1.00 | 22.24 | L | 0 |
| | ATOM | 1399 | CB | THR L | 180 | -16.510 | 21.437 | 108.450 | 1.00 | 24.69 | L | C |
| | ATOM | 1400 | OG1 | THR L | 180 | -15.554 | 21.720 | 107.419 | 1.00 | 28.70 | L | 0 |
| 25 | ATOM | 1401 | CG2 | THR L | 180 | -17.819 | 20.902 | 107.799 | 1.00 | 25.60 | L | C |
| | ATOM | 1402 | N | LEU L | 181 | -19.061 | 23.109 | 109.883 | 1.00 | 25.76 | L | N |
| | ATOM | 1403 | CA | LEU L | 181 | -20.256 | 23.079 | 110.722 | 1.00 | 23.80 | L | C |
| | ATOM | 1404 | C | LEU L | | -21.404 | 22.595 | 109.874 | 1.00 | 22.40 | L | С |
| | MOTA | 1405 | ŏ | | 181 | -21.281 | | 108.654 | 1.00 | 27.54 | L | 0 |
| 30 | MOTA | 1406 | СВ | LEU L | | -20.618 | | 111.158 | | 20.99 | L | C |
| 00 | MOTA | 1407 | CG | LEU L | | -19.507 | | 111.691 | | 21.11 | L | C |
| | MOTA | 1408 | | LEU L | | -19.910 | | 111.792 | | 18.26 | L | Č |
| | ATOM | 1409 | | LEU L | | -19.133 | | 113.056 | | 35.93 | _ L | Č |
| | MOTA | 1410 | N | THR L | | -22.537 | 22.342 | | | 21.49 | _ L | N |
| 35 | MOTA | 1411 | ČA | THR L | | -23.734 | | 109.771 | | 21.66 | L | Ċ |
| 33 | MOTA | 1412 | C | | 182 | ~24.299 | | 109.392 | | 18.67 | L L | č |
| | | 1413 | Ö | | 182 | -23.964 | | 110.009 | | 17.07 | Ŀ | õ |
| | ATOM | 1414 | CB | | 182 | -24.819 | | 110.648 | | 20.54 | L | č |
| | ATOM | 1415 | | | 182 | -25.233 | | 111.724 | | 19.08 | L | ŏ |
| 40 | MOTA | | OG1 | | 182 | -24.250 | | 111.210 | | 19.23 | L | č |
| 40 | ATOM | 1416 | CG2 | | 183 | -25.161 | | 108.377 | | 22.53 | L | N |
| | MOTA | 1417 | N | | | -25.817 | | 107.953 | | 27.93 | L | C |
| | ATOM | 1418 | CA | LYS L | | -26.611 | | 109.111 | | 28.40 | L | Č |
| | ATOM | 1419 | C | | 183 | | 26.367 | | | 28.75 | L | Õ |
| 4.5 | ATOM | 1420 | 0 | | 183 | -26.590 | | | | 24.85 | L L | C |
| 45 | ATOM | 1421 | CB | LYS L | | -26.777 | | 106.814 | | | | C |
| | MOTA | 1422 | CG | LYS L | | -27.654 | | 106.442 | | 38.68 | L | G |
| | MOTA | 1423 | CD | LYS L | | -28.739 | | 105.465 | | 51.46 | Ŀ | - |
| | ATOM | 1424 | CE | LYS L | 183 | -29.711 | | 105.066 | | 61.22 | L T | C |
| | MOTA | 1425 | NZ | LYS L | | -29.183 | | 103.976 | | 65.88 | L | N |
| 50 | MOTA | 1426 | N | ASP L | | -27.335 | | 109.825 | | 28.42 | L T | N |
| | ATOM | 1427 | CA | ASP L | | -28.132 | | 110.967 | 1.00 | 30.29 | L | C |
| | MOTA | 1428 | C | ASP L | | -27.275 | | 112.047 | | 27.78 | Ţ. | Ç |
| | MOTA | 1429 | 0 | ASP L | | -27.641 | | 112.605 | | 26.36 | L | 0 |
| | MOTA | 1430 | CB | ASP L | | -28.909 | | 111.550 | | 32.41 | L | C |
| 55 | MOTA | 1431 | CG | ASP L | | -30.029 | | 110.615 | | 47.03 | L | C |
| | MOTA | 1432 | OD1 | . ASP L | 184 | -30.432 | | 109.744 | | 50.38 | L | 0 |
| | MOTA | 1433 | OD2 | ASP L | 184 | -30.492 | | 110.752 | | 57.39 | L | 0 |
| | ATOM | 1434 | N | GLU L | 185 | -26.126 | | 112.341 | | 26.34 | L | N |
| | MOTA | 1435 | CA | GLU L | | -25.239 | 25.406 | 113.396 | | 22.33 | L | C |
| 60 | MOTA | 1436 | С | GLU L | 185 | -24.726 | 26.743 | 112.905 | 1.00 | 21.73 | L | C |
| | MOTA | 1437 | 0 | GLU L | 185 | -24.747 | 27.754 | 113.623 | 1.00 | 19.74 | L | 0 |
| | ATOM | 1438 | ĊВ | GLU L | | -24.076 | | 113.729 | 1.00 | 22.69 | L | C |
| | MOTA | 1439 | CG | GLU L | | -22.917 | | 114.549 | | 23.70 | L | C |
| | MOTA | 1440 | CD | GLU L | | -23.294 | | 116.017 | | 24.94 | L | Č |
| 65 | MOTA | 1441 | OE1 | | | -24.490 | | 116.384 | | 27.91 | L | Ö |
| | ATOM | 1442 | OE2 | | | -22.395 | | 116.802 | | 27.17 | L | Ö |
| | ATOM | 1443 | N | TYR L | | -24.296 | | 111.637 | | 20.59 | L | Ň |
| | MOTA | 1444 | CA | TYR L | | -23.812 | | 111.033 | | 20.72 | L | Ĉ |
| | ATOM | 1445 | C | TYR L | | -24.884 | | 111.135 | | 21.32 | L | č |
| | 2 2 T OLT | - 4 - 4 | _ | | | _ 1.501 | | | , | | | - |

| | ATOM ATOM | 1446 1447 | O TYR L 186 CB TYR L 186 | -24.594 -23.443 | 30.251 111.475 27.769 109.565 | 1.00 19.97 1.00 21.88 | L L | O C |
|----|--------------|---------------------|--------------------------------|--------------------|----------------------------------|--------------------------|----------------|--------|
| | ATOM | 1448 | CG TYR L 186 | -23.034 | 29.037 108.828 | 1.00 20.13 | L | С |
| | ATOM | 1449 | CD1 TYR L 186 | -21.856 | 29.713 109.171 | 1.00 16.10 | L | C |
| 5 | ATOM | 1450 | CD2 TYR L 186 | -23.841 | 29.589 107.835 | 1.00 13.47 | \mathbf{L} | C |
| | MOTA | 1451 | CE1 TYR L 186 | -21.492 | 30.928 108.541 | 1.00 22.60 | L | C |
| | ATOM | 1452 | CE2 TYR L 186 | -23.480 | 30.800 107.198 | 1.00 21.66 | L | C |
| | ATOM | 1453 | CZ TYR L 186 | -22.298 | 31.458 107.569 32.657 107.007 | 1.00 17.38 1.00 26.12 | L L | Ö |
| 10 | ATOM | 1454 1455 | OH TYR L 186 N GLU L 187 | -21.907 -26.145 | 28.732 110.882 | 1.00 26.58 | L | N |
| 10 | ATOM ATOM | 1456 | CA GLU L 187 | -27.213 | 29.744 110.959 | 1.00 28.79 | L | Ĉ |
| | MOTA | 1457 | C GLU L 187 | -27.671 | 30.156 112.367 | 1.00 26.96 | L | C |
| | ATOM | 1458 | O GLU L 187 | -28.433 | 31.112 112.532 | 1.00 28.18 | L | 0 |
| | MOTA | 1459 | CB GLU L 187 | -28.403 | 29.304 110.087 | 1.00 29.15 | ${f L}$ | С |
| 15 | ATOM | 1460 | CG GLU L 187 | -28.097 | 29.587 108.603 | 1.00 38.89 | Ļ | C |
| | MOTA | 1461 | CD GLU L 187 | -29.007 | 28.858 107.603 | 1.00 54.73 | L | C |
| | ATOM | 1462 | OE1 GLU L 187 | -28.892 | 29.178 106.397 | 1.00 54.75 1.00 57.19 | L L | 0 |
| | ATOM | 1463 | OE2 GLU L 187 N ARG L 188 | -29.806 -27.167 | 27.966 107.994 29.462 113.385 | 1.00 37.19 | L | И |
| 20 | ATOM ATOM | 1464 1465 | N ARG L 188 CA ARG L 188 | -27.107 | 29.793 114.769 | 1.00 23.86 | Ŀ | Ĉ |
| 20 | MOTA | 1466 | C ARG L 188 | -26.523 | 30.771 115.368 | 1.00 26.95 | Ŀ | Č |
| | ATOM | 1467 | O ARG L 188 | -26.692 | 31.203 116.517 | 1.00 32.94 | L | 0 |
| | MOTA | 1468 | CB ARG L 188 | -27.455 | 28.527 115.636 | 1.00 25.29 | L | C |
| | MOTA | 1469 | CG ARG L 188 | -28.633 | 27.610 115.410 | 1.00 18.49 | L | C |
| 25 | MOTA | 1470 | CD ARG L 188 | -28.685 | 26.568 116.464 | 1.00 20.66 | Ŀ | C |
| | ATOM | 1471 | NE ARG L 188 | -27.676 | 25.523 116.368 | 1.00 22.08 1.00 31.05 | L L | N C |
| | MOTA | 1472 | CZ ARG L 188 NH1 ARG L 188 | -27.839 -28.973 | 24.357 115.741 24.060 115.106 | 1.00 31.03 | L | N |
| | MOTA MOTA | $\frac{1473}{1474}$ | NH1 ARG L 188 NH2 ARG L 188 | -26.897 | 23.438 115.816 | 1.00 20.64 | Ŀ | N |
| 30 | ATOM | 1475 | N HIS L 189 | -25.492 | 31.149 114.613 | 1.00 27.14 | L | N |
| 00 | MOTA | 1476 | CA HIS L 189 | -24.505 | 32.053 115.171 | 1.00 23.85 | L | C |
| | MOTA | 1477 | C HIS L 189 | -24.228 | 33.199 114.218 | 1.00 24.26 | L | С |
| | MOTA | 1478 | O HIS L 189 | -24.560 | 33.131 113.040 | 1.00 20.63 | L | 0 |
| | MOTA | 1479 | CB HIS L 189 | -23.256 | 31.239 115.485 | 1.00 21.82 | Ŀ | C |
| 35 | MOTA | 1480 | CG HIS L 189 | -23.474 | 30.234 116.589 | 1.00 23.43 | L L | N C |
| | ATOM | 1481 | ND1 HIS L 189 | | 30.610 117.912 28.904 116.570 | 1.00 18.19 1.00 16.28 | r r | C |
| | ATOM ATOM | 1482 1483 | CD2 HIS L 189 CE1 HIS L 189 | | 29.561 118.670 | 1.00 13.06 | L | Č |
| | MOTA | 1484 | NE2 HIS L 189 | | 28.504 117.885 | 1.00 15.13 | L | N |
| 40 | ATOM | 1485 | N ASN L 190 | | 34.250 114.735 | 1.00 24.89 | L | N |
| | MOTA | 1486 | CA ASN L 190 | | 35.390 113.884 | 1.00 26.57 | L | С |
| | MOTA | 1487 | C ASN L 190 | | 35.834 113.572 | 1.00 25.07 | Ŀ | ď |
| | MOTA | 1488 | O ASN L 190 | | 36.240 112.473 | 1.00 18.65 | L | 0 |
| | ATOM | 1489 | CB ASN L 190 | | 36.593 114.472 | 1.00 33.07 1.00 44.22 | L L | C |
| 45 | MOTA | 1490 1491 | CG ASN L 190 OD1 ASN L 190 | | 37.786 113.535 37.657 112.341 | 1.00 44.22 | L | 0 |
| | ATOM ATOM | 1492 | ND2 ASN L 190 | | 38.956 114.065 | 1.00 38.66 | Ŀ | Ŋ |
| | MOTA | 1493 | N SER L 191 | | 35.798 114.568 | 1.00 24.96 | L | N |
| | MOTA | 1494 | CA SER L 191 | -19.696 | 36.279 114.426 | 1.00 24.15 | L | С |
| 50 | MOTA | 1495 | C SER L 191 | | 35.123 114.233 | 1.00 23.44 | L | C |
| | ATOM | 1496 | O SER L 191 | | | 1.00 25.33 | Ŀ | 0 |
| | MOTA | 1497 | CB SER L 191 | | 37.056 115.696 | 1.00 20.64 | L | C |
| | ATOM | 1498 | OG SER L 191 | | 37.707 115.570 35.164 113.130 | 1.00 34.95 1.00 20.47 | L L | N O |
| 55 | MOTA | 1499 1500 | N TYR L 192 CA TYR L 192 | | | 1.00 20.47 | L | Ç |
| 55 | ATOM ATOM | 1501 | C TYR L 192 | | 34.729 112.770 | 1.00 22.19 | Ŀ | č |
| | MOTA | 1502 | O TYR L 192 | | | 1.00 24.10 | L | 0 |
| | ATOM | 1503 | CB TYR L 192 | | | 1.00 17.62 | L | C |
| | MOTA | 1504 | CG TYR L 192 | -18.679 | | 1.00 23.22 | L | C |
| 60 | ATOM | 1505 | CD1 TYR L 192 | | | 1.00 22.59 | Ŀ | C |
| | MOTA | 1506 | CD2 TYR L 192 | | | 1.00 18.19 | L | C |
| | ATOM | 1507 | CE1 TYR L 192 | | | 1.00 18.75 | L _i | C |
| | MOTA | 1508 | CE2 TYR L 192 | | | 1.00 21.05 1.00 22.71 | L L | C |
| 65 | MOTA MOTA | 1509 1510 | CZ TYR L 192 OH TYR L 192 | | | 1.00 22.71 | L | ŏ |
| 00 | ATOM | 1511 | N THR L 193 | | | 1.00 22.36 | Ľ | N |
| | MOTA | 1512 | CA THR L 193 | | 34.774 113.604 | 1.00 24.41 | L | C |
| | MOTA | 1513 | C THR L 193 | -12.233 | 33.758 113.480 | 1.00 24.10 | L | C |
| | MOTA | 1514 | O THR L 193 | | 32.698 114.063 | 1.00 27.37 | L | 0 |

| | | ** ****** | | | | | | | |
|------|--------|-----------|--------------|-----|---------|----------------|------------|--------------|------|
| | ATOM | 1515 | CB THR L | 193 | -13.187 | 35.495 114.971 | 1.00 23.16 | L | С |
| | MOTA | 1516 | OG1 THR L | | -14.157 | 36.553 115.064 | 1.00 21.75 | L | ō |
| | | | CG2 THR L | | -11.784 | 36.009 115.147 | 1.00 24.75 | Ĺ | č |
| | MOTA | 1517 | | | | | | | |
| | ATOM | 1518 | M . CAR F | | -11.215 | 34.108 112.690 | 1.00 22.54 | L | N |
| 5 | MOTA | 1519 | CA CYS L | | -9.983 | 33.318 112.457 | 1.00 26.58 | L | C |
| | MOTA | 1520 | C CYS L | 194 | -8.897 | 34.154 113.238 | 1.00 26.19 | L | C |
| | MOTA | 1521 | O CYS L | 194 | -8.706 | 35.294 112.848 | 1.00 24.23 | L | 0 |
| | | 1522 | • | | -9.561 | 33.391 110.919 | 1.00 24.94 | L | č |
| | ATOM | | | | | | | | |
| | MOTA | 1523 | SG CYS L | | -8.068 | 32.434 110.661 | 1.00 42.81 | L | S |
| 10 | MOTA | 1524 | N GLU L | | -8.283 | 33.639 114.320 | 1.00 24.48 | L | N |
| | MOTA | 1525 | CA GLU L | 195 | -7.182 | 34.334 115.024 | 1.00 29.59 | \mathbf{L} | C |
| | ATOM | 1526 | C GLU L | 195 | -5.844 | 33.609 114.798 | 1.00 30.32 | L | C |
| | ATOM | 1527 | O GLU L | | -5.736 | 32.409 115.054 | 1.00 32.34 | L | ŏ |
| | | | | | -7.426 | 34.400 116.545 | 1.00 32.34 | Ĺ | |
| | MOTA | 1528 | | | | | | | C |
| 15 | ATOM | 1529 | CG GLU L | | -8.541 | 35.343 116.918 | 1.00 36.24 | L | C |
| | ATOM | 1530 | CD GLU L | 195 | -8.662 | 35.481 118.422 | 1.00 40.41 | L | C |
| | MOTA | 1531 | OE1 GLU L | 195 | -7.813 | 34.889 119.126 | 1.00 37.64 | L | 0 |
| | MOTA | 1532 | OE2 GLU L | | -9.588 | 36.176 118.878 | 1.00 45.58 | L | 0 |
| | ATOM | 1533 | N ALA L | | -4.832 | 34.351 114.356 | 1.00 29.64 | L | Ň |
| 00 | | | | | | | 1.00 28.09 | L | |
| 20 | MOTA | 1534 | CA ALA L | | -3.507 | 33.789 114.084 | | | Ç |
| | MOTA | 1535 | C ALA L | | -2.409 | 34.420 114.908 | 1.00 28.54 | L | C |
| | ATOM | 1536 | O ALA L | | -2.284 | 35.642 114.929 | 1.00 30.56 | L | 0 |
| | ATOM | 1537 | CB ALA L | 196 | -3.153 | 33.991 112.624 | 1.00 29.68 | L | C |
| | ATOM | 1538 | N THR L | | -1.607 | 33.592 115.568 | 1.00 29.39 | L | N |
| 25 | ATOM | 1539 | CA THR L | | -0.473 | 34.125 116.305 | 1.00 32.75 | L | Ċ |
| 25 | | | | | | | | | |
| | ATOM | 1540 | C THR L | | 0.759 | 33.583 115.564 | 1.00 31.12 | Ŀ | Ğ |
| | MOTA | 1541 | O THR L | | 0.832 | 32.420 115.140 | 1.00 28.19 | L | 0 |
| | MOTA | 1542 | CB THR L | 197 | -0.477 | 33.711 117.796 | 1.00 34.20 | \mathbf{L} | C |
| | ATOM | 1543 | OG1 THR L | 197 | -0.216 | 32.310 117.927 | 1.00 37.75 | L | 0 |
| 30 | ATOM | 1544 | CG2 THR L | | -1.827 | 34.046 118.406 | 1.00 33.92 | L | Ċ |
| 30 | | | | | 1.711 | 34.469 115.370 | 1.00 30.73 | L | N |
| | MOTA | 1545 | N HIS L | | | | | | |
| | MOTA | 1546 | CA HIS L | | 2.919 | 34.147 114.605 | 1.00 27.74 | L | C |
| | ATOM | 1547 | C HIS L | 198 | 4.036 | 34.915 115.289 | 1.00 28.66 | L | C |
| | MOTA | 1548 | O HIS L | 198 | 3.788 | 35.879 116.009 | 1.00 26.28 | L | 0 |
| 35 | ATOM | 1549 | CB HIS L | 198 | 2.719 | 34.651 113.168 | 1.00 24.97 | L | С |
| 00 | MOTA | 1550 | CG HIS L | | 3.864 | 34.340 112.254 | 1.00 23.60 | L | č |
| | | | | | | | | | |
| | ATOM | 1551 | ND1 HIS L | | 4.789 | 35.292 111.880 | 1.00 26.74 | L, | N |
| | MOTA | 1552 | CD2 HIS L | | 4.259 | 33.179 111.670 | 1.00 23.17 | L | С |
| | MOTA | 1553 | CE1 HIS L | 198 | 5.706 | 34.729 111.110 | 1.00 22.18 | L | C |
| 40 | MOTA | 1554 | NE2 HIS L | 198 | 5.410 | 33.448 110.968 | 1.00 17.91 | L | N |
| | MOTA | 1555 | N LYS L | | 5.268 | 34.499 115.058 | 1.00 28.46 | L | N |
| | MOTA | 1556 | CA LYS L | | 6.391 | 35.179 115.711 | 1.00 30.45 | ī | Ĉ |
| | | | | | | | | L | |
| | MOTA | 1557 | C LYS L | | 6.336 | 36.684 115.519 | 1.00 30.56 | | G |
| | MOTA | 1558 | O LYS L | | 6.784 | 37.429 116.387 | 1.00 34.50 | L | 0 |
| 45 | MOTA | 1559 | CB LYS L | 199 | 7.707 | 34.633 115.116 | 1.00 31.22 | L | С |
| | MOTA | 1560 | CG LYS L | 199 | 9.034 | 35.296 115.576 | 1.00 33.02 | L | C |
| | MOTA | 1561 | CD LYS L | | | 34.717 114.743 | 1.00 31.75 | L | C |
| | | 1562 | CE LYS L | | 11.548 | 35.183 115.205 | 1.00 26.57 | Ē | č |
| | ATOM | | CE 1110 I | 100 | | 24 725 114 206 | 1.00 25.57 | | |
| | ATOM | 1563 | NZ LYS L | | 12.553 | 34.725 114.206 | | Ŀ | N |
| 50 | MOTA | 1564 | N THR L | | 5.783 | 37.135 114.393 | 1.00 30.74 | L | N |
| | ATOM | 1565 | CA THR L | 200 | 5.785 | 38.554 114.042 | 1.00 30.39 | L | C |
| | MOTA | 1566 | C THR L | 200 | 4.916 | 39.445 114.890 | 1.00 36.75 | I, | C |
| | ATOM | 1567 | O THR L | | 4.831 | 40.651 114.626 | 1.00 40.22 | L | 0 |
| | | 1568 | CB THR L | | 5.430 | 38.783 112.541 | 1.00 30.63 | L | č |
| | MOTA | | | | | | | | |
| 55 | MOTA | 1569 | OG1 THR L | | 4.283 | 37.982 112.176 | 1.00 34.17 | Ļ | 0 |
| | MOTA | 1570 | CG2 THR L | 200 | 6.642 | 38.347 111.650 | 1.00 26.33 | L | C |
| | MOTA | 1571 | N SER L | 201 | 4.240 | 38.842 115.875 | 1.00 42.72 | L | N |
| | MOTA | 1572 | CA SER L | | 3.444 | 39.601 116.831 | 1.00 43.91 | L | C |
| | ATOM | 1573 | C SER L | | 2.855 | 38.728 117.916 | 1.00 47.57 | L | Ċ |
| 60 | | | | | | | | | ~ |
| 60 | ATOM | 1574 | O SER L | | 2.126 | 37.756 117.644 | 1.00 50.70 | L | 0 |
| | MOTA | 1575 | CB SER L | | 2.328 | 40.364 116.130 | 1.00 43.23 | L | C |
| | ATOM | 1576 | OG SER L | | 1.711 | 41.223 117.077 | 1.00 48.62 | L | 0 |
| | ATOM | 1577 | N THR L | | 3.160 | 39.073 119.157 | 1.00 52.05 | L | N |
| | ATOM | 1578 | CA THR L | | 2.652 | 38.344 120.314 | 1.00 56.48 | Ī. | Ĉ |
| G.E. | | | | | | | | | G |
| 65 | MOTA | 1579 | C THR L | | 1.097 | 38.311 120.322 | 1.00 56.15 | Ŀ | |
| | ATOM | 1580 | O THR L | | 0.468 | 37.332 120.756 | 1.00 56.79 | Ļ | 0 |
| | MOTA | 1581 | CB THR L | 202 | 3.147 | 39.041 121.586 | 1.00 59.00 | L | C |
| | MOTA | 1582 | OG1 THR L | | 4.517 | 39.445 121.400 | 1.00 62.75 | L | . O. |
| | MOTA | 1583 | CG2 THR L | | 3.065 | 38.103 122.770 | 1.00 63.28 | L | C |
| | WI OIL | 7000 | ~~~ 1111\ JJ | | 2.003 | JULIU IIII 170 | | | _ |

| | | 4504 | | | 000 | 0 404 | 20 200 110 04 | - 4 00 54 07 | - | 37 |
|-----|-----------------|------|------------------|---------|-----|---------|----------------|--------------|--------|--------------------------|
| | ATOM | 1584 | N | SER L | | 0.494 | 39.399 119.845 | | Ţ | $\widetilde{\mathbf{N}}$ |
| | MOTA | 1585 | CA | SER L | | -0.965 | 39.544 119.772 | | L | C |
| | MOTA | 1586 | C | | 203 | -1.454 | 38.958 118.442 | | L | С |
| | ATOM | 1587 | 0 | SER L | 203 | -0.916 | 39.279 117.37 | | L | 0 |
| 5 | MOTA | 1588 | CB | SER L | 203 | -1.298 | 41.013 119.79 | 1 1.00 54.28 | L | С |
| | MOTA | 1589 | OG | SER L | 203 | -0.510 | 41.642 118.792 | 2 1.00 58.41 | L | 0 |
| | MOTA | 1590 | N | PRO L | 204 | -2.522 | 38.151 118.47 | 7 1.00 47.34 | L | N |
| | ATOM | 1591 | . CA | PRO L | | -3.014 | 37.553 117.233 | | L | С |
| | ATOM | 1592 | C | PRO L | | -3.502 | 38.506 116.169 | | L | Č |
| 10 | MOTA | 1593 | Ö | | 204 | -3.898 | 39.613 116.45 | | - L | Õ |
| 10 | | 1594 | | PRO L | | -4.137 | 36.635 117.71 | | r L | č |
| | ATOM | | CB | | | | | | L | G |
| | MOTA | 1595 | CG | PRO L | | -4.723 | - , | | | |
| | MOTA | 1596 | $^{\rm CD}$ | PRO L | | -3.435 | 37.849 119.59 | | Ţ | C |
| | MOTA | 1597 | И | ILE L | | -3.460 | 38.043 114.92 | | L | N |
| 15 | ATOM | 1598 | $^{\mathrm{ca}}$ | ILE L | | -3.986 | 38.796 113.78 | | L | C |
| | \mathbf{MOTA} | 1599 | С | ILE L | | -5.428 | 38.239 113.75 | | L | C |
| | MOTA | 1600 | 0 | ILE L | 205 | -5.641 | 37.013 113.78 | | L | 0 |
| | MOTA | 1601 | CB | ILE L | 205 | -3.219 | 38.432 112.47 | 1 1.00 34.55 | L | C |
| | ATOM | 1602 | CG1 | ILE L | 205 | -1.814 | 39.073 112.50 | 3 1.00 31.34 | L | C |
| 20 | MOTA | 1603 | CG2 | ILE L | 205 | -3.974 | 38.938 111.24 | 8 1.00 24.01 | L | C |
| | ATOM | 1604 | CD1 | | | -0.939 | 38.666 111.29 | 0 1.00 42.44 | L | С |
| | ATOM | 1605 | N | VAL L | | -6.396 | 39.139 113.73 | | L | N |
| | ATOM | 1606 | CA | VAL L | | -7.813 | 38.759 113.78 | | L | C |
| | MOTA | 1607 | C | VAL L | | -8.582 | 39.102 112.52 | | L | č |
| OE. | | 1608 | Ö | VAL L | | -8.531 | 40.234 112.08 | | Ŀ | ŏ |
| 25 | ATOM | | | VAL L | | -8.485 | 39.495 115.01 | | L | č |
| | ATOM | 1609 | CB | | | | | | L | |
| | MOTA | 1610 | | VAL L | | -9.979 | 39.144 115.10 | | | C |
| | MOTA | 1611 | | VAL L | | -7.782 | 39.060 116.32 | | L | C |
| | MOTA | 1612 | N | LYS L | | -9.259 | 38.127 111.90 | | L | N |
| 30 | MOTA | 1613 | ca | LYS L | | -10.088 | 38.410 110.71 | | Ŀ | C |
| | MOTA | 1614 | C | | | -11.472 | 37.832 111.03 | | L | C |
| | MOTA | 1615 | 0 | LYS L | | -11.585 | 36.737 111.56 | | · L | 0 |
| | ATOM | 1616 | CB | LYS L | 207 | -9.560 | 37.756 109.45 | 0 1.00 23.08 | L | C |
| | MOTA | 1617 | CG | LYS L | 207 | -8.259 | 38.397 109.00 | 2 1.00 32.25 | L | C |
| 35 | MOTA | 1618 | CD | LYS L | 207 | -8.452 | 39.818 108.44 | 4 1.00 39.96 | L | C |
| | MOTA | 1619 | CE | LYS L | | -7.059 | 40.481 108.24 | 5 1.00 45.64 | L | C |
| | ATOM | 1620 | NZ | LYS L | | -7.248 | 41.837 107.67 | | L | N |
| | MOTA | 1621 | N | SER L | | -12.515 | 38.553 110.69 | | L | N |
| | MOTA | 1622 | CA | SER L | | -13.865 | 38.071 111.04 | | L | Ċ |
| 40 | ATOM | 1623 | CA | SER L | | -14.875 | 38.506 110.05 | | L | č |
| 40 | | | | SER L | | -14.619 | 39.407 109.26 | | L | ŏ |
| | MOTA | 1624 | 0 | | | | | | L | č |
| | MOTA | 1625 | CB | SER L | | -14.363 | | | | |
| | MOTA | 1626 | OG | SER L | | -13.384 | 38.712 113.36 | | L | 0 |
| | ATOM | 1627 | N | PHE L | | -16.051 | 37.880 110.10 | | L | |
| 45 | MOTA | 1628 | CA | PHE L | | -17.173 | 38.342 109.30 | | L | C |
| | MOTA | 1629 | C | PHE L | 209 | -18.428 | 38.049 110.12 | | L | C |
| | MOTA | 1630 | 0 | PHE L | | -18.387 | 37.253 111.05 | | L | 0 |
| | MOTA | 1631 | CB | PHE L | 209 | -17.269 | 37.664 107.93 | 9 1.00 16.13 | L | С |
| | MOTA | 1632 | CG | PHE L | 209 | -17.620 | 36.198 108.00 | 0 1.00 26.94 | L | |
| 50 | MOTA | 1633 | CD1 | PHE L | 209 | -18.955 | 35.765 108.03 | 9 1.00 26.84 | L | С |
| | ATOM | 1634 | CD2 | | | -16.606 | 35.241 108.00 | 0 1.00 31.15 | L | C |
| | MOTA | 1635 | | PHE L | | -19.254 | 34.404 108.07 | 2 1.00 27.00 | 上 | C |
| | MOTA | 1636 | CE2 | | | -16.897 | 33.895 108.02 | | L | |
| | ATOM | 1637 | CZ | PHE L | | -18.229 | 33.464 108.06 | | L | |
| 55 | ATOM | 1638 | N | ASN L | | -19.522 | 38.737 109.81 | | L | |
| 55 | | | CA | ASN L | | -20.809 | 38.497 110.47 | | L | |
| | MOTA | 1639 | | | | | 37.868 109.43 | | L | |
| | ATOM | 1640 | C | ASN L | | -21.715 | | | | |
| | ATOM | 1641 | 0 | ASN L | | -21.804 | 38.326 108.30 | | L | |
| | MOTA | 1642 | CB | ASN L | | -21.424 | 39.789 110.98 | | Ŀ | |
| 60 | MOTA | 1643 | CG | ASN L | | -20.647 | 40.358 112.13 | 1 1.00 41.97 | Ĩ, | |
| | MOTA | 1644 | | . ASN L | | -20.232 | 39.624 113.02 | | L | |
| | ATOM | 1645 | ND2 | ASN L | 210 | -20.427 | 41.673 112.11 | | L | |
| | MOTA | 1646 | N | ARG L | 211 | -22.349 | 36.779 109.81 | 0 1.00 34.50 | L | |
| | MOTA | 1647 | CA | ARG L | 211 | -23.225 | 36.076 108.89 | | L | |
| 65 | ATOM | 1648 | C | ARG L | | -24.255 | 37.088 108.36 | | L | |
| | ATOM | 1649 | Ó | ARG L | | -24.483 | 37.085 107.12 | 9 1.00 47.09 | L | |
| | MOTA | 1650 | ČВ | ARG L | | -23.897 | 34.874 109.60 | | L | C |
| | MOTA | 1651 | CG | ARG L | | -24.800 | 33.985 108.72 | | L | |
| | ATOM | 1652 | CD | ARG L | | -25.278 | 32.779 109.47 | | L | |
| | | | | | | | | | | |

| | - 5024 | 1.650 | 3.777 | 3 D.C. T | 011 | 05 000 | 22 106 | 110 705 | 1 00 30 30 | т | ВT |
|----|--------------|--------------|----------|----------------|-------------|-----------------------|------------------|--------------------|--------------------------|--------|--------|
| | MOTA | 1653 1654 | CZ NE | ARG L ARG L | | -25.888 -27.142 | | 110.725 110.849 | 1.00 38.28 1.00 44.67 | L | N C |
| | ATOM ATOM | 1655 | | ARG L | | -27.142 | | 109.786 | 1.00 48.24 | L | N |
| | ATOM | 1656 | NH2 | | 211 | -27.568 | | 112.027 | 1.00 46.31 | L | N |
| 5 | ATOM | 1657 | | ARG L | | -24.796 | | 109.158 | 1.00 43.58 | Ē | õ |
| Ü | TER | 1658 | Q | | 211 | 21.75 | | | | _ | _ |
| | MOTA | 1659 | N | GLU H | 1 | 13.634 | 16.019 | 73.396 | 1.00 37.05 | н | N |
| | ATOM | 1660 | CA | GLU H | 1 | 13.497 | 15.897 | 74.879 | 1.00 37.26 | H | C |
| | MOTA | 1661 | С | GLU H | 1 | 12.992 | 14.523 | 75.281 | 1.00 32.62 | H | С |
| 10 | MOTA | 1662 | 0 | GLU H | 1 | 12.103 | 13.972 | 74.644 | 1.00 31.05 | H | 0 |
| | ATOM | 1663 | CB | GLU H | 1 | 12.537 | 16.969 | 75.411 | 1.00 39.07 | H | C |
| | MOTA | 1664 | CG | GLU H | 1 | 11.930 | 16.635 | 76.750 | 1.00 56.68 | Н | C |
| | MOTA | 1665 | CD | GLU H | 1 | 11.585 | 17.889 | 77.553 | 1.00 73.84 | H | C |
| | MOTA | 1666 | | GLU H | 1 | 11.488 | 17.807 | 78.805 | 1.00 77.86 | H | 0 |
| 15 | ATOM | 1667 | OE2 | | 1 | 11.417 | 18.958 | 76.922 | 1.00 78.38 1.00 30.97 | H | O |
| | MOTA | 1668 | N | H JAV | 2 | 13.548 13.122 | 13.973 12.653 | 76.355 76.833 | 1.00 30.97 | H H | C N |
| | MOTA ATOM | 1669 1670 | CA C | VAL H | 2 2 | 11.817 | 12.857 | 77.557 | 1.00 25.45 | H | č |
| | ATOM | 1671 | Ö | VAL H | 2 | 11.670 | 13.778 | 78.359 | 1.00 28.52 | H | ŏ |
| 20 | MOTA | 1672 | ČВ | VAL H | 2 | 14.101 | 12.061 | 77.867 | 1.00 21.49 | H | č |
| | ATOM | 1673 | | VAL H | 2 | 13.467 | 10.846 | 78.519 | 1.00 20.68 | Н | Ċ |
| | ATOM | 1674 | CG2 | VAL H | 2 | 15.439 | 11.700 | 77.205 | 1.00 23.15 | H | С |
| | MOTA | 1675 | N | ALA H | 3 | 10.865 | 11.994 | 77.290 | 1.00 25.40 | H | N |
| | MOTA | 1676 | CA | ALA H | 3 | 9.593 | 12.073 | 77.975 | 1.00 28.29 | H | С |
| 25 | MOTA | 1677 | C | ALA H | 3 | 9.089 | 10.661 | 78.373 | 1.00 26.97 | H | C |
| | ATOM | 1678 | 0 | ALA H | 3 | 9.185 | 9.698 | 77.593 | 1.00 29.48 | H | 0 |
| | MOTA | 1679 | CB | ALA H | 3 | 8.549 | 12.845 | 77.052 | 1.00 27.69 | H | C |
| | MOTA | 1680 | N | LEU H | 4 | 8.609 8.061 | 10.538 9.287 | 79.612 80.137 | 1.00 24.22 1.00 20.89 | H H | C N |
| 30 | ATOM | 1681 1682 | CA C | LEU H | 4 4 | 6.689 | 9.658 | 80.678 | 1.00 20.89 | H | Č |
| 30 | MOTA MOTA | 1683 | Ö | LEU H | 4 | 6.584 | 10.514 | 81.590 | 1.00 27.07 | H | ŏ |
| | ATOM | 1684 | СВ | LEU H | 4 | 8.916 | 8.766 | 81.302 | 1.00 22.55 | H | Ğ |
| | ATOM | 1685 | CG | LEU H | $\tilde{4}$ | 10.384 | 8.474 | 80.837 | 1.00 17.66 | H | Ċ |
| | ATOM | 1686 | | LEU H | 4 | 11.151 | 8.000 | 82.071 | 1.00 17.39 | H | С |
| 35 | MOTA | 1687 | CD2 | LEU H | 4 | 10.446 | 7.366 | 79.750 | 1.00 23.92 | H | C |
| | MOTA | 1688 | N | VAL H | 5 | 5.639 | 9.005 | 80.176 | 1.00 24.40 | H | N |
| | ATOM | 1689 | CA | VAL H | -5 | 4.290 | 9.364 | 80.620 | 1.00 20.43 | H | C |
| | MOTA | 1690 | C | VAL H | 5 | 3.513 | 8.155 | 81.167 | 1.00 20.69 | H | Č |
| | MOTA | 1691 | 0_ | VAL H | 5 | 3.095 | 7.262 | 80.397 | 1.00 23.26 | H | 0 |
| 40 | ATOM | 1692 | CB | VAL H | 5 | 3.505 | 9.990 10.282 | 79.464 | 1.00 17.37 1.00 12.65 | H H | C C |
| | MOTA ATOM | 1693 1694 | | VAL H | 5 5 | $\frac{2.092}{4.204}$ | 11.263 | 79.925 78.989 | 1.00 12.03 | H | ä |
| | ATOM | 1695 | N CGZ | GLU H | 6 | 3.282 | 8.143 | 82.474 | 1.00 18.23 | H | Ŋ |
| | ATOM | 1696 | CA | GLU H | 6 | 2.590 | 6.997 | 83.074 | 1.00 21.02 | H | Ĉ |
| 45 | MOTA | 1697 | C | GLU H | 6 | 1.080 | 7.101 | 83.005 | 1.00 24.64 | H | C |
| | ATOM | 1698 | Ō | GLU H | 6 | 0.535 | 8.187 | 82.930 | 1.00 24.72 | H | 0 |
| | MOTA | 1699 | CB | GLU H | 6 | 2.948 | 6.778 | 84.539 | 1.00 23.51 | H | C |
| | MOTA | 1700 | CG | GLU H | 6 | 4.498 | 6.643 | 84.825 | 1.00 22.40 | H | C |
| | MOTA | 1701 | CD | GLU H | 6 | 5.121 | 7.975 | 85.129 | 1.00 24.00 | H | Č |
| 50 | MOTA | 1702 | OE1 | | 6 | 4.652 | 9.035 | 84.652 | 1.00 22.51 | H | 0 |
| | ATOM | 1703 | OE2 | | 6 | 6.169 | 7.956 | 85.930 82.993 | 1.00 20.14 1.00 25.35 | H H | O |
| | MOTA | 1704 | N | SER H | 7 7 | 0.426 -1.051 | 5.954 5.957 | 83.008 | 1.00 23.33 | H | N C |
| | MOTA MOTA | 1705 1706 | CA C | SER H SER H | | -1.494 | 4.639 | 83.623 | 1.00 23.70 | H | g |
| 55 | ATOM | 1707 | Ö | SER H | | -0.669 | 3.750 | 83.870 | 1.00 23.79 | H | ŏ |
| 00 | ATOM | 1708 | СВ | SER H | | -1.625 | 6.137 | 81.602 | 1.00 24.31 | H | č |
| | MOTA | 1709 | OG | SER H | | -1.219 | 5.109 | 80.733 | 1.00 29.67 | H | 0 |
| | ATOM | 1710 | N | GLY H | 8 | -2.793 | 4.535 | 83.926 | 1.00 24.57 | H | N |
| | MOTA | 1711 | CA | GLY H | 8 | -3.309 | 3.306 | 84.479 | 1.00 26.40 | H | C |
| 60 | MOTA | 1712 | С | GLY H | | -3.483 | 3.239 | 85.973 | 1.00 27.67 | H | C |
| | MOTA | 1713 | 0 | GLY H | | -3.994 | 2.242 | 86.485 | 1.00 32.68 | H | 0 |
| | ATOM | 1714 | N | GLY H | | -3.071 | 4.256 | 86.714 | 1.00 26.70 | H | N |
| | MOTA | 1715 | CA | GLY H | | -3.267 | 4.106 | 88.133 | 1.00 30.26 1.00 31.53 | H H | C |
| 65 | MOTA | 1716 1717 | C O | GLY H | | -4.736 -5.554 | $4.366 \\ 4.742$ | 88.505 87.658 | 1.00 34.39 | H | Ö |
| UO | MOTA MOTA | 1718 | N | GLY H | | -5.050 | 4.186 | 89.771 | 1.00 26.64 | H | И |
| | MOTA | 1719 | CA | GLY H | | -6.399 | 4.406 | 90.224 | 1.00 24.06 | H | Ĉ |
| | MOTA | 1720 | C | GLY H | | -6.617 | 3.606 | 91.474 | 1.00 28.46 | H | č |
| | ATOM | 1721 | Ö | GLY H | | -5.670 | 3.135 | 92.107 | 1.00 29.65 | H | 0 |
| | | | | | | | | | | | |

| | * | | | | | | | | | | |
|----|-----------------|------|-----------|-----------------|--------|----------|---------|------------|---|--------|---|
| | MOTA | 1722 | N LEU H | 11 | -7.89 | 3.418 | 91.830 | 1.00 27.81 | | H | N |
| | MOTA | 1723 | CA LEÙ H | 11 | -8.24 | | 93.050 | 1.00 26.68 | | H | Ċ |
| | ATOM | 1724 | C LEU H | 11 | -8.46 | | 92.762 | 1.00 29.79 | | H | č |
| | MOTA | 1725 | O LEU H | 11 | -9.13 | | 91.790 | 1.00 23.73 | | | |
| 5 | ATOM | 1726 | CB LEU H | 11 | | | | | | H | 0 |
| 3 | | | | | -9.55 | | 93.616 | 1.00 27.46 | | H | C |
| | ATOM | 1727 | CG LEU H | 11 | -10.21 | | 94.829 | 1.00 30.78 | | H | С |
| | MOTA | 1728 | CD1 LEU H | 11 | -9.38 | | 96.069 | 1.00 21.39 | | H | C |
| | MOTA | 1729 | CD2 LEU H | 11 | -11.57 | | 95.076 | 1.00 26.61 | | H | C |
| | MOTA | 1730 | N VAL H | 12 | -7.97 | 0.362 | 93.641 | 1.00 31.51 | | H | N |
| 10 | MOTA | 1731 | CA VAL H | 12 | -8.14 | -1.062 | 93.408 | 1.00 31.17 | | H | C |
| | MOTA | 1732 | C VAL H | 12 | -8.34 | | 94.747 | 1.00 29.15 | | H | č |
| | MOTA | 1733 | O VAL H | 12 | -7.77 | | 95.722 | 1.00 29.56 | | H | |
| | | 1734 | | | | | | | | | 0 |
| | MOTA | | CB VAL H | 12 | -6.87 | | 92.693 | 1.00 32.00 | | H | C |
| | MOTA | 1735 | CG1 VAL H | 12 | -5.59 | | 93.539 | 1.00 28.63 | | H- | C |
| 15 | MOTA | 1736 | CG2 VAL H | 12 | -7.04 | | 92.482 | 1.00 29.00 | | H | C |
| | MOTA | 1737 | N LYS H | 13 | -9.17 | 5 -2.723 | 94.826 | 1.00 28.70 | | H | N |
| | MOTA | 1738 | CA LYS H | 13 | -9.36 | 3 -3.342 | 96.115 | 1.00 31.56 | | H | C |
| | MOTA | 1739 | C LYS H | 13 | -8.21 | -4.272 | 96.474 | 1.00 30.38 | | H | Č |
| | MOTA | 1740 | O LYS H | 13 | -7.51 | | 95.618 | 1.00 33.11 | | H | õ |
| 20 | MOTA | 1741 | CB LYS H | 13 | -10.69 | | 96.145 | 1.00 33.11 | | | |
| 20 | ATOM | 1742 | | 13 | | | | | | H | C |
| | | | | | -11.89 | | 95.773 | 1.00 41.91 | | H | C |
| | MOTA | 1743 | CD LYS H | 13 | -13.18 | | 96.279 | 1.00 51.54 | | H | C |
| | MOTA | 1744 | CE LYS H | 13 | -14.38 | | 95.690 | 1.00 65.14 | | H | C |
| | MOTA | 1745 | NZ LYS H | 13 | -14.44 | 7 ~3.378 | 94.190 | 1.00 58.25 | | H | N |
| 25 | MOTA | 1746 | N PRO H | 14 | -8.00 | 5 -4.494 | 97.763 | 1.00 28.47 | | H | N |
| | MOTA | 1747 | CA PRO H | 14 | -6.93 | 5 -5.398 | 98.191 | 1.00 27.81 | | H | C |
| | MOTA | 1748 | C PRO H | 14 | -7.15 | | 97,499 | 1.00 30.73 | | H | č |
| | ATOM | 1749 | O PRO H | $\frac{14}{14}$ | -8.30 | | 97.382 | 1.00 33.00 | | H | ŏ |
| | ATOM | 1750 | CB PRO H | 14 | -7.16 | | 99.686 | 1.00 27.15 | | H | č |
| 30 | ATOM | 1751 | | | | | | | | | |
| 30 | | | CG PRO H | 14 | -7.81 | | 100.033 | 1.00 25.33 | | H | C |
| | ATOM | 1752 | CD PRO H | 14 | -8.68 | | 98.901 | 1.00 24.23 | | H | C |
| | MOTA | 1753 | N GLY H | 15 | -6.07 | | 97.087 | 1.00 31.50 | | H | N |
| | MOTA | 1754 | CA GLY H | 15 | -6.14 | -8.694 | 96.398 | 1.00 26.43 | | H | C |
| | MOTA | 1755 | C GLY H | 15 | -6.40 | 2 -8.471 | 94.922 | 1.00 31.35 | | H | C |
| 35 | MOTA | 1756 | O GLY H | 15 | -6.34 | 3 -9.393 | 94.114 | 1.00 37.77 | | H | 0 |
| | MOTA | 1757 | N GLY H | 16 | -6.65 | | 94.547 | 1.00 30.42 | | H | N |
| | MOTA | 1758 | CA GLY H | 16 | -6.92 | | 93.159 | 1.00 30.36 | | H | Ĉ |
| | ATOM | 1759 | C GLY H | 16 | -5.67 | | 92.275 | 1.00 30.40 | | H | Č |
| | MOTA | 1760 | O GLY H | 16 | -4.55 | | 92.740 | | | | |
| 40 | | | | | | | | 1.00 33.82 | | H | 0 |
| 40 | ATOM | 1761 | N SER H | 17 | -5.91 | | 91.007 | 1.00 27.09 | | H | N |
| | MOTA | 1762 | CA SER H | 17 | -4.89 | | 89.970 | 1.00 31.01 | | H | C |
| | MOTA | 1763 | C SER H | 17 | -5.03 | | 89.249 | 1.00 33.12 | | H | C |
| | \mathbf{MOTA} | 1764 | O SER H | 17 | -6.11 | 3 ~4.506 | 89.210 | 1.00 35.49 | | H | 0 |
| | MOTA | 1765 | CB SER H | 17 | -5.03 | -7.527 | 88.925 | 1.00 29.40 | | Ħ | C |
| 45 | MOTA | 1766 | OG SER H | 17 | -4.51 | -8.733 | 89.433 | 1.00 40.23 | | H | 0 |
| | MOTA | 1767 | N LEU H | 18 | -3.93 | | 88.635 | 1.00 29.11 | | H | Ň |
| | MOTA | 1768 | CA LEU H | 18 | -3.96 | | 87.892 | 1.00 31.40 | | H | Ĉ |
| | MOTA | 1769 | C LEU H | 18 | -2.73 | | 86.979 | 1.00 28.04 | | H | Č |
| | ATOM | 1770 | O LEU H | 18 | -1.70 | | 87.384 | 1.00 28.04 | | | |
| 50 | | | | | | | | | | H | 0 |
| 50 | ATOM | 1771 | CB LEU H | 18 | -3.90 | | 88.882 | 1.00 36.05 | | H | С |
| | MOTA | 1772 | CG LEU H | 18 | -4.09 | | 88.311 | 1.00 36.13 | | H | C |
| | MOTA | 1773 | CD1 LEU H | 18 | -5.51 | | 87.716 | 1.00 32.11 | | H | С |
| | MOTA | 1774 | CD2 LEU H | 18 | -3.91 | 0.228 | 89.402 | 1.00 41.12 | | H | C |
| | MOTA | 1775 | N LYS H | 19 | -2.83 | 3 -2.822 | 85.789 | 1.00 23.49 | | H | N |
| 55 | MOTA | 1776 | CA LYS H | 19 | -1.67 | | 84.915 | 1.00 23.15 | | H | Ĉ |
| | ATOM | 1777 | C LYS H | 19 | -1.35 | | 84.578 | 1.00 26.43 | | H | Č |
| | ATOM | 1778 | O LYS H | 19 | -2.20 | | | | | | |
| | | | | | | | 84.062 | 1.00 25.06 | | H | 0 |
| | ATOM | 1779 | CB LYS H | 19 | -1.91 | | 83.593 | 1.00 24.43 | | H | C |
| | ATOM | 1780 | CG LYS H | 19 | -0.62 | | 82.771 | 1.00 28.16 | | H | C |
| 60 | MOTA | 1781 | CD LYS H | 19 | -0.87 | | 81.551 | 1.00 27.11 | | H | C |
| | MOTA | 1782 | CE LYS H | 19 | 0.438 | | 80.971 | 1.00 37.87 | | H | C |
| | MOTA | 1783 | NZ LYS H | 19 | 0.22 | 7 ~5.854 | 79.670 | 1.00 50.80 | : | H | N |
| | MOTA | 1784 | N LEU H | 20 | -0.120 | | 84.881 | 1.00 25.63 | | H | N |
| | ATOM | 1785 | CA LEU H | 20 | 0.33 | | 84.587 | 1.00 23.09 | | H | C |
| 65 | MOTA | 1786 | C LEU H | 20 | 1.119 | | 83.293 | 1.00 21.89 | | H | č |
| | MOTA | 1787 | O LEU H | 20 | 1.81 | | 82.969 | 1.00 23.58 | | H | ŏ |
| | ATOM | 1788 | CB LEU H | 20 | 1.27 | | 85.707 | 1.00 23.38 | | n H | Ċ |
| | ATOM | 1789 | CG LEU H | 20 | 0.799 | | 87.143 | 1.00 22.80 | | | Č |
| | | | | | | | | | | H | C |
| | ATOM | 1790 | CD1 LEU H | 20 | 1.85 | 1.306 | 88.119 | 1.00 30.17 |] | H | C |

| | MOTA | 1791 | CD2 | LEU H | 20 | -0.538 | 1.505 | 87.267 | 1.00 26.07 | H | С |
|-----|-----------------|------|--------------|-------|----|--------|--------|--------|------------|---|--------|
| | ATOM | 1792 | N | SER H | 21 | 1.050 | 1.558 | 82.595 | 1.00 19.29 | H | Ŋ |
| | | | | | | | | - | 1.00 22.08 | | |
| | MOTA | 1793 | CA | SER H | 21 | 1.749 | 1.754 | 81.359 | | H | C |
| | MOTA | 1794 | С | SER H | 21 | 2.636 | 2.978 | 81.440 | 1.00 24.30 | H | С |
| 5 | ATOM | 1795 | 0 | SER H | 21 | 2.353 | 3.911 | 82.195 | 1.00 27.22 | H | 0 |
| • | ATOM | 1796 | ČВ | SER H | 21 | 0.748 | 1.964 | 80.229 | 1.00 21.00 | H | č |
| | | | | | | | | | | | |
| | ATOM | 1797 | QG | SER H | 21 | 0.011 | 0.761 | 80.030 | 1.00 34.43 | H | 0 |
| | \mathbf{MOTA} | 1798 | N | CYS H | 22 | 3.661 | 2.991 | 80.608 | 1.00 21.98 | H | N |
| | MOTA | 1799 | CA | CYS H | 22 | 4.571 | 4.125 | 80.536 | 1.00 20.64 | н | C |
| 40 | | | | | 22 | 4.981 | 4.313 | 79.090 | 1.00 21.24 | | |
| 10 | ATOM | 1800 | C | CYS H | | | | | | H | Ç |
| | MOTA | 1801 | 0 | CYS H | 22 | 5.646 | 3.437 | 78.532 | 1.00 27.26 | H | 0 |
| | ATOM | 1802 | CB | CYS H | 22 | 5.802 | 3.897 | 81.424 | 1.00 21.02 | H | С |
| | ATOM | 1803 | SG | CYS H | 22 | 6.992 | 5.249 | 81.188 | 1.00 29.58 | H | s |
| | | | | | | | | | | | |
| | MOTA | 1804 | N | ALA H | 23 | 4.556 | 5.436 | 78.489 | 1.00 17.76 | H | N |
| 15 | MOTA | 1805 | ca | ALA H | 23 | 4.855 | 5.821 | 77.114 | 1.00 20.00 | H | C |
| | MOTA | 1806 | С | ALA H | 23 | 6.179 | 6.585 | 77.077 | 1.00 23.26 | H | С |
| | ATOM | 1807 | ŏ | ALA H | 23 | 6.306 | 7.663 | 77.655 | 1.00 25.72 | H | ŏ |
| | | | | | | | | | | | |
| | MOTA | 1808 | CB | ALA H | 23 | 3.739 | 6.738 | 76.544 | 1.00 17.81 | H | C |
| | \mathbf{MOTA} | 1809 | \mathbf{N} | ALA H | 24 | 7.133 | 6.073 | 76.318 | 1.00 24.36 | H | N |
| 20 | MOTA | 1810 | CA | ALA H | 24 | 8.427 | 6.705 | 76.290 | 1.00 25.28 | H | C |
| | ATOM | 1811 | C | ALA H | 24 | 8.741 | 7.270 | 74.950 | 1.00 26.13 | H | č |
| | | | | | | | | | | | |
| | MOTA | 1812 | 0 | ALA H | 24 | 8.397 | 6.679 | 73.921 | 1.00 27.39 | H | 0 |
| | MOTA | 1813 | CB | ALA H | 24 | 9.480 | 5.704 | 76.687 | 1.00 25.98 | H | C |
| | MOTA | 1814 | N | SER H | 25 | 9.407 | 8.414 | 74.946 | 1.00 24.17 | H | N |
| 25 | ATOM | 1815 | CA | SER H | 25 | 9.761 | 9.022 | 73.680 | 1.00 26.47 | H | |
| 25 | | | | | | | | | | | |
| | MOTA | 1816 | С | SER H | 25 | 11.004 | 9.896 | 73.855 | 1.00 26.46 | H | |
| | MOTA | 1817 | 0 | SER H | 25 | 11.383 | 10.242 | 74.967 | 1.00 28.62 | H | 0 |
| | MOTA | 1818 | CB | SER H | 25 | 8.583 | 9.889 | 73.200 | 1.00 27.45 | H | C |
| | | 1819 | | SER H | 25 | 8.344 | 10.935 | 74.132 | 1.00 24.69 | H | |
| | MOTA | | OG | | | | | | | | - |
| 30 | MOTA | 1820 | N | GLY H | 26 | 11.678 | 10.210 | 72.769 | 1.00 22.55 | H | N |
| | MOTA | 1821 | CA | GLY H | 26 | 12.807 | 11.111 | 72.911 | 1.00 20.54 | H | С |
| | MOTA | 1822 | С | GLY H | 26 | 14.151 | 10.470 | 73.084 | 1.00 24.32 | Ħ | C |
| | | | | | | | | 73.294 | 1.00 24.89 | H | Õ |
| | MOTA | 1823 | 0 | GLY H | 26 | 15.139 | 11.176 | | | | |
| | MOTA | 1824 | N | PHE H | 27 | 14.199 | 9.141 | 73.028 | 1.00 21.93 | H | |
| 35 | MOTA | 1825 | CA | PHE H | 27 | 15.482 | 8.426 | 73.112 | 1.00 20.14 | H | С |
| | MOTA | 1826 | C | PHE H | 27 | 15.297 | 7.067 | 72.471 | 1.00 21.32 | н | C |
| | | | | | | | | | | | |
| | MOTA | 1827 | 0 | PHE H | 27 | 14.152 | 6.622 | 72.250 | 1.00 23.00 | H | 0 |
| | ATOM | 1828 | $^{\rm CB}$ | PHE H | 27 | 15.964 | 8.301 | 74.591 | 1.00 20.36 | H | |
| | MOTA | 1829 | CG | PHE H | 27 | 15.035 | 7.491 | 75.504 | 1.00 18.12 | H | C |
| 40 | MOTA | 1830 | | PHE H | 27 | 15.278 | 6.164 | 75.788 | 1.00 10.19 | H | |
| 40 | | | | | | | | 76.058 | | | |
| | MOTA | 1831 | CD2 | | 27 | 13.905 | 8.073 | | 1.00 18.20 | H | |
| | ATOM | 1832 | CE1 | PHE H | 27 | 14.417 | 5.404 | 76.613 | 1.00 15.96 | H | |
| | MOTA | 1833 | CE2 | PHE H | 27 | 13.028 | 7.329 | 76.893 | 1.00 21.16 | H | C |
| | ATOM | 1834 | CZ | PHE H | 27 | 13.276 | 6.009 | 77.174 | 1.00 9.67 | H | Ċ |
| 45 | | | | | | | | | | | |
| 45 | MOTA | 1835 | N | THR H | 28 | 16.400 | 6.358 | 72.225 | 1.00 20.96 | H | |
| | MOTA | 1836 | ca | THR H | 28 | 16.307 | 5.056 | 71.570 | 1.00 20.74 | H | С |
| | MOTA | 1837 | С | THR H | 28 | 15.937 | 4.013 | 72.549 | 1.00 22.28 | H | C |
| | MOTA | 1838 | Ō | THR H | 28 | 16.775 | 3.363 | 73.126 | 1.00 25.49 | H | |
| | | | | | | | | | | | |
| | MOTA | 1839 | СВ | THR H | 28 | 17.610 | 4.727 | 70.871 | 1.00 17.35 | H | C |
| 50 | MOTA | 1840 | OG1 | THR H | 28 | 17.834 | 5.747 | 69.902 | 1.00 22.02 | H | 0 |
| | MOTA | 1841 | CG2 | THR H | 28 | 17.527 | 3.399 | 70.157 | 1.00 21.93 | H | C |
| | MOTA | 1842 | N | PHE H | 29 | 14.636 | 3.854 | 72.730 | 1.00 20.12 | H | |
| | | | | | | | 3.034 | 72.750 | | | |
| | MOTA | 1843 | CA | PHE H | 29 | 14.092 | 2.922 | 73.707 | 1.00 19.24 | H | |
| | MOTA | 1844 | С | PHE H | 29 | 14.698 | 1.534 | 73.827 | 1.00 20.34 | H | C |
| 55 | MOTA | 1845 | 0 | PHE H | 29 | 15.023 | 1.081 | 74.937 | 1.00 22.88 | H | 0 |
| - | MOTA | 1846 | ČВ | PHE H | 29 | 12.568 | 2.808 | 73.476 | 1.00 18.98 | H | |
| | | | | | | | | | | | č |
| | MOTA | 1847 | CG | PHE H | 29 | 11.821 | 2.069 | 74.551 | 1.00 18.94 | H | |
| | MOTA | 1848 | CD1 | PHE H | 29 | 11.547 | 2.681 | 75.784 | 1.00 17.20 | H | |
| | MOTA | 1849 | CD2 | | 29 | 11.337 | 0.774 | 74.328 | 1.00 17.93 | H | C |
| 60 | MOTA | 1850 | CE1 | | 29 | 10.802 | 1.996 | 76.752 | 1.00 20.22 | H | |
| 00 | | | | | | | | | | | \sim |
| | MOTA | 1851 | CE2 | | 29 | 10.587 | 0.086 | 75.316 | 1.00 20.54 | H | |
| | MOTA | 1852 | CZ | PHE H | 29 | 10.330 | 0.704 | 76.515 | 1.00 7.20 | H | C |
| | MOTA | 1853 | N | ILE H | 30 | 14.872 | 0.847 | 72.699 | 1.00 22.05 | H | |
| | MOTA | 1854 | CA | ILE H | 30 | 15.393 | -0.520 | 72.753 | 1.00 24.80 | H | |
| GE. | | | | | | | | | | | ~ |
| 65 | ATOM | 1855 | С | ILE H | 30 | 16.752 | -0.688 | 73.403 | 1.00 22.06 | H | |
| | MOTA | 1856 | 0 | ILE H | 30 | 17.027 | -1.775 | 73.909 | 1.00 23.49 | H | |
| | MOTA | 1857 | CB | ILE H | 30 | 15.488 | -1.222 | 71.350 | 1.00 23.26 | H | |
| | ATOM | 1858 | CG1 | | 30 | 16.369 | -0.396 | 70.424 | 1.00 23.10 | H | |
| | | | | | | | | | | | |
| | ATOM | 1859 | CG2 | ILE H | 30 | 14.061 | -1.412 | 70.768 | 1.00 32.12 | H | С |

| | T CM | 1060 | CD1 TTE H | 30 | 16.802 | -1.136 | 69.186 | 1.00 38.83 | Н | С |
|----|--------------|--------------|------------------------|----------|------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM ATOM | 1860 1861 | CD1 ILE H N SER H | 31 | 17.546 | 0.377 | 73.443 | 1.00 18.26 | - H | N |
| | MOTA | 1862 | CA SER H | 31 | 18.890 | 0.261 | 74.003 | 1.00 18.45 1.00 18.69 | H H | C C |
| _ | MOTA MOTA | 1863 1864 | C SER H O SER H | 31 31 | 18.984 20.041 | 0.503 0.256 | 75.508 76.089 | 1.00 21.46 | H | Ö |
| 5 | ATOM | 1865 | CB SER H | 31 | 19.874 | 1.206 | 73.291 | 1.00 14.50 | H | C |
| | ATOM | 1866 | OG SER H | 31 | 20.169 | 0.722 | 71.962 | 1.00 31.45 | H | N |
| | MOTA | 1867 | N TYR H | 32 32 | 17.883 17.886 | $0.952 \\ 1.240$ | 76.124 77.549 | 1.00 18.03 1.00 14.33 | H H | C |
| 10 | ATOM ATOM | 1868 1869 | CA TYR H C TYR H | 32 32 | 17.152 | 0.280 | 78.441 | 1.00 15.02 | H | Č |
| 10 | MOTA | 1870 | O TYR H | 32 | 16.115 | -0.302 | 78.076 | 1.00 14.37 | H | 0 |
| | ATOM | 1871 | CB TYR H | 32 | 17.310 | 2.665 | 77.818 | 1.00 13.79 1.00 17.16 | H H | C |
| | ATOM | 1872 | CG TYR H CD1 TYR H | 32 32 | 18.198 18.203 | 3.793 4.142 | 77.298 75.943 | 1.00 17.10 | H | C |
| 15 | MOTA MOTA | 1873 1874 | CD1 TYR H CD2 TYR H | 32 | 19.042 | 4.487 | 78.156 | 1.00 14.56 | Н | C |
| 13 | ATOM | 1875 | CE1 TYR H | 32 | 19.020 | 5.152 | 75.457 | 1.00 17.45 | H | C |
| | MOTA | 1876 | CE2 TYR H | 32 | 19.882 | 5.505 | 77.679 | 1.00 20.18 1.00 23.49 | H H | C |
| | ATOM | 1877 | CZ TYR H | 32 32 | 19.857 20.666 | 5.828 6.850 | 76.330 75.863 | 1.00 23.49 | Н | ŏ |
| 20 | MOTA MOTA | 1878 1879 | OH TYR H N ALA H | 33 | 17.698 | 0.140 | 79.651 | 1.00 14.42 | H | N |
| 20 | ATOM | 1880 | CA ALA H | 33 | 17.057 | -0.615 | 80.695 | 1.00 14.51 | H | C |
| | MOTA | 1881 | C ALA H | 33 | 15.993 | 0.394 | 81.252 | 1.00 14.39 1.00 12.17 | H H | O C |
| | ATOM | 1882 | O ALA H CB ALA H | 33 33 | 16.123 18.055 | 1.624 -1.001 | 81.104 81.806 | 1.00 12.17 | H | č |
| 25 | MOTA MOTA | 1883 1884 | CB ALA H N MET H | 34 | 14.949 | -0.140 | 81.862 | 1.00 16.84 | H | N |
| 20 | MOTA | 1885 | CA MET H | 34 | 13.874 | 0.700 | 82.416 | 1.00 16.36 | H | C |
| | MOTA | 1886 | C MET H | 34 | 13.439 | 0.188 | 83.758 84.086 | 1.00 15.55 1.00 13.11 | H H | O C |
| | ATOM | 1887 1888 | O MET H CB MET H | 34 34 | 13.601 12.651 | -0.987 0.697 | 81.474 | 1.00 15.11 | H | ç |
| 30 | ATOM ATOM | 1889 | CG MET H | 34 | 12.887 | 1.223 | 80.071 | 1.00 14.09 | H | C |
| 00 | ATOM | 1890 | SD MET H | 34 | 13.108 | 3.014 | 79.968 | 1.00 20.48 | H | S |
| | MOTA | 1891 | CE MET H | 34 | 11.533 | 3.688 1.053 | 80.662 84.546 | 1.00 7.18 1.00 16.91 | H H | C N |
| | MOTA | 1892 1893 | N SER H CA SER H | 35 35 | 12.790 12.374 | 0.616 | 85.875 | 1.00 19.04 | H | ĉ |
| 35 | ATOM ATOM | 1894 | C SER H | 35 | 11.092 | 1.306 | 86.348 | 1.00 18.31 | H | C |
| 00 | ATOM | 1895 | O SER H | 35 | 10.620 | 2.251 | 85.722 | 1.00 24.04 | H | 0 |
| | MOTA | 1896 | CB SER H | 35 | 13.451 | 0.992 | 86.951 86.723 | 1.00 14.30 1.00 22.00 | H H | C |
| | MOTA | 1897 1898 | OG SER H N TRP H | 35 36 | 14.755 10.567 | 0.386 0.771 | 87.440 | 1.00 12.01 | H | Ň |
| 40 | MOTA MOTA | 1899 | CA TRP H | 36 | 9.448 | 1.383 | 88.154 | 1.00 12.95 | H | C |
| 40 | ATOM | 1900 | C TRP H | 36 | 9.970 | 1.598 | 89.590 | 1.00 18.28 | H | C C |
| | ATOM | 1901 | O TRP H | 36 | 10.611 8.232 | 0.709 0.467 | 90.210 88.231 | 1.00 16.01 1.00 14.71 | H H | G |
| | MOTA MOTA | 1902 1903 | CB TRP H | 36 36 | 7.503 | 0.323 | 86.885 | 1.00 21.41 | H | C |
| 45 | ATOM | 1904 | CD1 TRP H | 36 | 7.705 | ~0.669 | 85.937 | 1.00 9.67 | H | C |
| | MOTA | 1905 | CD2 TRP H | | 6.505 | 1.203 | 86.345 | 1.00 18.07 1.00 23.74 | H H | C N |
| | MOTA | 1906 | | 36 36 | 6.897 6.144 | -0.430 0.698 | 84.856 85.078 | 1.00 23.74 | H | Ç |
| | MOTA MOTA | 1907 1908 | CE2 TRP H CE3 TRP H | | 5.874 | 2.365 | 86.817 | 1.00 4.98 | H | C |
| 50 | ATOM | 1909 | CZ2 TRP H | | 5.177 | 1.314 | 84.267 | 1.00 16.74 | H | C |
| | MOTA | 1910 | CZ3 TRP H | | 4.929 | 2.981 2.456 | 86.022 84.745 | 1.00 19.83 1.00 18.46 | H H | C |
| | MOTA | 1911 1912 | CH2 TRP H N VAL H | | 4.582 9.660 | 2.430 | 90.138 | 1.00 19.29 | H | N |
| | MOTA MOTA | 1913 | CA VAL H | | 10.093 | 3.115 | 91.481 | 1.00 19.64 | H | C |
| 55 | MOTA | 1914 | | 37 | 8.845 | 3.770 | 92.101 | 1.00 19.14 | H | C |
| | ATOM | 1915 | | | 8.269 | 4.629 4.180 | 91.495 91.436 | 1.00 19.32 1.00 20.61 | H H | 0 |
| | ATOM | 1916 1917 | | | 11.249 11.648 | 4.586 | 92.880 | 1.00 17.50 | H | Č |
| | ATOM ATOM | 1918 | | | 12.488 | 3.563 | 90.693 | 1.00 17.13 | H | C |
| 60 | ATOM | 1919 | N ARG H | 38 | 8.492 | 3.378 | 93.319 | 1.00 16.77 | H | N |
| | MOTA | 1920 | | | 7.287 7.630 | 3.953 4.775 | 93.923 95.146 | 1.00 15.98 1.00 18.04 | H H | C |
| | MOTA | 1921 1922 | | | 8.684 | 4.773 | | 1.00 16.62 | H | Ο. |
| | ATOM ATOM | 1923 | | | 6.282 | 2.840 | 94.307 | 1.00 16.85 | H | С |
| 65 | ATOM | 1924 | CG ARG H | 38 | 6.772 | 1.938 | | 1.00 8.21 | H H | C C |
| | MOTA | 1925 | | | 5.789 6.272 | 0.730 -0.154 | | 1.00 11.19 1.00 14.89 | H | И |
| | MOTA MOTA | 1926 1927 | | | 5.688 | -1.319 | | 1.00 22.76 | H | C |
| | MOTA | 1928 | | | 4.620 | -1.693 | | 1.00 24.06 | H | N |

| | ATOM | 1929 | NH2 ARG H | 38 | 6.132 | -2.078 97.948 | 1.00 23.16 | Н | N |
|----|--------------|--------------|------------------------|----------|-----------------------|---------------------------------|--------------------------|--------|--------|
| | MOTA | 1930 1931 | N GLN H CA GLN H | 39 39 | 6.722 6.952 | 5.687 95.494 6.530 96.674 | 1.00 18.48 1.00 22.51 | H H | N C |
| | ATOM ATOM | 1932 | CA GLN H | 39 | 5.681 | 6.398 97.560 | 1.00 26.22 | H | č |
| 5 | ATOM | 1933 | O GLN H | 39 | 4.589 | 6.703 97.106 | 1.00 29.41 | H | 0 |
| | MOTA | 1934 1935 | CB GLN H CG GLN H | 39 39 | 7.135 7.516 | 7.993 96.242 8.855 97.445 | 1.00 20.08 1.00 14.71 | H H | C |
| | ATOM ATOM | 1936 | CG GLN H CD GLN H | 39 | 8.012 | 10.206 97.003 | 1.00 17.69 | H | Č |
| | ATOM | 1937 | OE1 GLN H | 39 | 7.450 | 10.799 96.080 | 1.00 22.74 | H | 0 |
| 10 | ATOM | 1938 | NE2 GLN H | 39 | 9.069 | 10.709 97.657 5.960 98.790 | 1.00 18.94 1.00 25.08 | H H | N |
| | ATOM ATOM | 1939 1940 | N THR H CA THR H | 40 40 | 5.873 4.759 | 5.695 99.685 | 1.00 25.08 | H | C |
| | MOTA | 1941 | C THR H | 40 | 4.186 | 6.999 100.217 | 1.00 33.51 | H | C |
| | MOTA | 1942 | O THR H | 40 | 4.780 | 8.083 100.063 | 1.00 32.02 | H | 0 |
| 15 | ATOM ATOM | 1943 1944 | CB THR H OG1 THR H | 40 40 | 5.216 6.209 | 4.895 100.892 5.658 101.561 | 1.00 31.26 1.00 31.13 | H H | C O |
| | ATOM | 1945 | CG2 THR H | 40 | 5.773 | 3.512 100.514 | 1.00 25.76 | H | č |
| | MOTA | 1946 | N PRO H | 41 | 3.022 | 6.913 100.873 | 1.00 36.66 | H | N |
| 00 | ATOM | 1947 | CA PRO H | 41 41 | 2.477 3.443 | 8.172 101.383 8.778 102.402 | 1.00 36.86 1.00 34.19 | H H | C |
| 20 | ATOM ATOM | 1948 1949 | C PRO H O PRO H | 41 | 3.458 | 9.974 102.614 | 1.00 34.19 | H | Õ |
| | ATOM | 1950 | CB PRO H | 41 | 1.129 | 7.754 101.986 | 1.00 37.38 | H | C |
| | ATOM | 1951 | CG PRO H | 41 | 0.734 | 6.506 101.085 5.790 101.047 | 1.00 40.44 1.00 34.79 | H H | C C |
| 25 | MOTA MOTA | 1952 1953 | CD PRO H N GLU H | 41 42 | 2.088 4.267 | 7.959 103.020 | 1.00 34.79 | H | И |
| 20 | ATOM | 1954 | CA GLU H | 42 | 5.212 | 8.508 103.978 | 1.00 31.61 | H | С |
| | MOTA | 1955 | C GLU H | 42 | 6.439 | 9.112 103.280 | 1.00 30.07 | H H | C |
| | MOTA MOTA | 1956 1957 | O GLU H CB GLU H | 42 42 | 7.333 5.637 | 9.576 103.954 7.449 104.982 | 1.00 28.54 1.00 35.54 | H H | C O |
| 30 | ATOM | 1958 | CG GLU H | 42 | 4.441 | 6.687 105.587 | 1.00 46.36 | Н | С |
| | MOTA | 1959 | CD GLU H | 42 | 3.822 | 5.712 104.591 | 1.00 59.41 | н | C |
| | ATOM | 1960 1961 | OE1 GLU H OE2 GLU H | 42 42 | $\frac{4.424}{2.748}$ | 4.635 104.358 6.039 104.027 | 1.00 59.82 1.00 63.05 | H H | 0 |
| | ATOM ATOM | 1962 | N LYS H | 43 | 6.428 | 9.133 101.944 | 1.00 25.52 | H | N |
| 35 | MOTA | 1963 | CA LYS H | 43 | 7.505 | 9.712 101.126 | 1.00 24.37 | H | C |
| | ATOM | 1964 | C LYS H | 43 43 | 8.755 9.754 | 8.881 100.935 9.391 100.407 | 1.00 24.96 1.00 22.88 | H H | C C |
| | ATOM ATOM | 1965 1966 | O LYS H CB LYS H | 43 | 7.938 | 11.087 101.655 | 1.00 27.09 | H | č |
| | MOTA | 1967 | CG LYS H | 43 | 7.326 | 12.215 100.938 | 1.00 34.74 | H | C |
| 40 | MOTA | 1968 | CD LYS H | 43 | 5.872 | 12.299 101.209 | 1.00 51.35 1.00 51.99 | H H | C C |
| | MOTA MOTA | 1969 1970 | CE LYS H NZ LYS H | 43 43 | 5.123 3.689 | 12.594 99.921 12.833 100.223 | 1.00 51.99 1.00 50.46 | H | N |
| | MOTA | 1971 | N ARG H | 44 | 8.717 | 7.612 101.318 | 1.00 25.07 | H | N |
| | MOTA | 1972 | CA ARG H | 44 | 9.917 | 6.778 101.151 | 1.00 27.51 | H | C C |
| 45 | ATOM ATOM | 1973 1974 | C ARG H O ARG H | 44 44 | 9.887 8.816 | 6.273 99.709 5.960 99.168 | 1.00 27.18 1.00 23.86 | H H | 0 |
| | ATOM | 1975 | CB ARG H | 44 | 9.897 | 5.561 102.080 | 1.00 30.75 | H | Č |
| | ATOM | 1976 | CG ARG H | 44 | 9.672 | 5.841 103.567 | 1.00 44.30 | H | C |
| 50 | MOTA | 1977 1978 | CD ARG H NE ARG H | 44 44 | 10.839 12.097 | 6.497 104.317 5.755 104.254 | 1.00 61.82 1.00 70.52 | H H | C N |
| 50 | ATOM ATOM | 1979 | CZ ARG H | 44 | 13.093 | 5.869 105.139 | 1.00 63.42 | H | C |
| | MOTA | 1980 | NH1 ARG H | 44 | 12.985 | 6.684 106.193 | 1.00 51.27 | H | N |
| | MOTA | 1981 | NH2 ARG H | 44 | 14.233 11.057 | 5.217 104.925 6.234 99.095 | 1.00 41.30 1.00 21.99 | H H | N N |
| 55 | MOTA MOTA | 1982 1983 | N LEU H | 45 45 | 11.181 | 5.768 97.723 | 1.00 23.75 | H | C |
| | MOTA | 1984 | C LEU H | 45 | 11.637 | 4.287 97.779 | 1.00 22.20 | H | C |
| | ATOM | 1985 | O LEU H | 45 | 12.519 | 3.933 98.550 | 1.00 21.33 1.00 20.46 | H H | С О |
| | MOTA MOTA | 1986 1987 | CB LEU H CG LEU H | 45 45 | 12.238 11.743 | 6.607 96.978 8.037 96.592 | 1.00 26.46 | Ħ | C |
| 60 | MOTA | 1988 | CD1 LEU H | 45 | 12.981 | 8.967 96.324 | 1.00 19.17 | H | C |
| | MOTA | 1989 | CD2 LEU H | 45 | 10.849 | 8.021 95.337 | 1.00 7.95 | H | C |
| | ATOM ATOM | 1990 1991 | N GLUH CA GLUH | 46 46 | 11.037 11.398 | 3.465 96.940 2.041 96.915 | 1.00 21.98 1.00 26.58 | H H | С |
| | ATOM | 1992 | C GLU H | 46 | 11.450 | 1.571 95.478 | 1.00 21.11 | H | č |
| 65 | MOTA | 1993 | O GLU H | 46 | 10.467 | 1.731 94.751 | 1.00 22.21 | H | 0 |
| | ATOM | 1994 | CB GLU H | 46 46 | 10.311 10.123 | 1.189 97.635 1.593 99.117 | 1.00 28.65 1.00 49.98 | H H | C C |
| | ATOM ATOM | 1995 1996 | CD GLU H | 46 46 | 8.955 | 0.846 99.817 | 1.00 49.98 | H | C |
| | ATOM | 1997 | OE1 GLU H | 46 | 8.157 | 0.180 99.090 | 1.00 54.94 | H | 0 |
| | | | | | 142 | | | | |
| | | | | | | | | | |

| | ATOM | 1998 | OE2 | GLU H | 46 | 8.861 | | 101.080 | 1.00 76.63 | H | |
|----|--------------|--------------|------------|----------------|----------|------------------|------------------|------------------|--------------------------|--------|-----|
| • | MOTA ATOM | 1999 2000 | N CA | TRP H | 47 47 | 12.586 12.708 | $1.015 \\ 0.485$ | 95.071 93.728 | 1.00 16.27 1.00 17.07 | H | |
| | ATOM | 2001 | C | TRP H | 47 | 11.769 | -0.762 | 93.679 | 1.00 15.27 | H | C C |
| 5 | ATOM ATOM | 2002 2003 | O CB | TRP H | 47 47 | 11.792 14.181 | -1.584 0.092 | 94.592 93.501 | 1.00 18.79 1.00 19.17 | H | |
| | MOTA | 2003 | CG | TRP H | 47 | 14.181 | -0.878 | 92.324 | 1.00 19.17 | H | |
| | MOTA | 2005 | | TRP H | 47 | 14.232 | -0.609 | 90.978 | 1.00 8.71 | H | C C |
| 10 | MOTA MOTA | 2006 2007 | CD2 NE1 | TRP H | 47 47 | 14.708 14.425 | -2.240 -1.758 | 92.432 90.246 | 1.00 15.94 1.00 15.37 | H H | |
| 10 | ATOM | 2007 | CE2 | TRP H | 47 | 14.728 | -2.771 | 91.121 | 1.00 13.37 | H | |
| | MOTA | 2009 | CE3 | TRP H | 47 | 14.987 | -3.087 | 93.520 | 1.00 19.49 | H | C C |
| | MOTA MOTA | 2010 2011 | CZ2 CZ3 | TRP H TRP H | 47 47 | 15.021 15.280 | -4.120 -4.440 | 90.864 93.257 | 1.00 17.65 1.00 11.79 | H | |
| 15 | ATOM | 2012 | CH2 | TRP H | 47 | 15.293 | -4.929 | 91.945 | 1.00 16.64 | H | |
| | MOTA | 2013 | N | VAL H | 48 | 10.976 | -0.857 | 92.613 | 1.00 16.40 | H | I N |
| | MOTA MOTA | 2014 2015 | CA C | VAL H VAL H | 48 48 | 9.980 10.328 | -1.935 -2.961 | 92.400 91.316 | 1.00 20.27 1.00 17.27 | H | |
| | MOTA | 2016 | ŏ | VAL H | 48 | 9.966 | -4.116 | 91.442 | 1.00 17.49 | H | |
| 20 | MOTA | 2017 | CB | VAL H | 48 | 8.602 | -1.279 | 92.038 | 1.00 21.34 | H | C C |
| | MOTA MOTA | 2018 2019 | | VAL H VAL H | 48 48 | 7.611 8.052 | -2.301 -0.607 | 91.498 93.274 | 1.00 24.15 1.00 24.24 | H H | _ |
| | MOTA | 2020 | N | ALA H | 49 | 11.034 | -2.548 | 90.263 | 1.00 16.96 | H | |
| 05 | ATOM | 2021 | CA | ALA H | 49 | 11.346 | -3.493 | 89.194 | 1.00 17.77 | H | |
| 25 | MOTA MOTA | 2022 2023 | C O | ALA H ALA H | 49 49 | 12.206 12.109 | -2.877 -1.657 | 88.154 87.912 | 1.00 19.92 1.00 24.74 | H H | |
| | MOTA | 2024 | CB | ALA H | 49 | 10.021 | -3.962 | 88.495 | 1.00 16.94 | H | r C |
| | ATOM ATOM | 2025 2026 | N CA | SER H SER H | 50 50 | 12.980 13.807 | -3.721 -3.266 | 87.465 86.363 | 1.00 21.88 1.00 21.57 | H H | |
| 30 | MOTA | 2027 | C | SER H | 50 | 13.754 | -4.316 | 85.265 | 1.00 21.78 | H | |
| | ATOM | 2028 | 0 | SER H | 50 | 13.545 | -5.502 | 85.563 | 1.00 23.60 | H | 0 |
| | MOTA MOTA | 2029 2030 | CB OG | SER H SER H | 50 50 | 15.272 15.460 | -3.137 -2.078 | 86.774 87.683 | 1.00 21.45 1.00 21.58 | H H | |
| | MOTA | 2031 | N | ILE H | 51 | 13.900 | -3.849 | 84.036 | 1.00 20.05 | H | |
| 35 | MOTA | 2032 | CA | ILE H | 51 | 14.003 | ~4.754 | 82.858 | 1.00 17.96 | H | |
| | MOTA MOTA | 2033 2034 | C O | ILE H | 51 51 | 15.172 15.269 | -4.273 -3.087 | 81.999 81.682 | 1.00 17.53 1.00 19.16 | H H | _ |
| | ATOM | 2035 | СВ | ILE H | 51 | 12.679 | -4.795 | 82.058 | 1.00 17.66 | H | t C |
| 40 | ATOM ATOM | 2036 2037 | CG1 CG2 | | 51 51 | 12.796 12.325 | ~5.869 ~3.407 | 80.958 81.427 | 1.00 23.68 1.00 8.10 | H H | |
| 40 | ATOM | 2038 | CD1 | | 51 | 11.433 | -6.214 | 80.376 | 1.00 15.41 | H | |
| | ATOM | 2039 | N | SER H | 52 | 16.100 | -5.176 | 81.625 | 1.00 14.90 | H | |
| | ATOM ATOM | 2040 2041 | CA C | SER H SER H | 52 52 | 17.264 16.899 | -4.790 -4.630 | 80.816 79.352 | 1.00 15.78 1.00 16.46 | H | _ |
| 45 | MOTA | 2042 | ō | SER H | 52 | 15.815 | -5.022 | 78.940 | 1.00 22.00 | H | |
| | ATOM ATOM | 2043 2044 | CB OG | SER H | 52 52 | 18.384 17.962 | -5.853 -7.063 | 80.913 | 1.00 15.21 | H | |
| | ATOM | 2045 | N | SER H SER H | 53 | 17.786 | -4.068 | 80.253 78.558 | 1.00 20.35 1.00 18.03 | H | |
| | ATOM | 2046 | CA | SER H | 53 | 17.515 | ~3.925 | 77.129 | 1.00 20.13 | H | T C |
| 50 | ATOM ATOM | 2047 2048 | С О | SER H SER H | 53 53 | 17.441 16.774 | -5.342 -5.539 | 76.528 75.518 | 1.00 22.74 1.00 26.71 | H H | |
| | MOTA | 2049 | CB | SER H | 53 | 18.645 | -3.160 | 76.445 | 1.00 20.15 | H | |
| | ATOM | 2050 | OG | SER H | 53 | 19.898 | -3.829 | 76.632 | 1.00 16.33 | H | |
| 55 | MOTA MOTA | 2051 2052 | N CA | GLY H | 54 54 | 18.102 18.041 | -6.314 -7.697 | 77.160 76.676 | 1.00 22.48 1.00 18.24 | H H | |
| | MOTA | 2053 | C | GLY H | 54 | 16.805 | -8.441 | 77.176 | 1.00 22.94 | H | |
| | ATOM | 2054 | O | GLY H | 54 | 16.562 | ~9.593 | 76.800 | 1.00 22.69 | H | |
| | MOTA ATOM | 2055 2056 | N CA | GLY H | 55 55 | 16.017 14.806 | -7.799 -8.434 | 78.044 78.547 | 1.00 20.19 1.00 15.12 | H | |
| 60 | ATOM | 2057 | C | GLY H | 55 | 14.880 | -9.146 | 79.888 | 1.00 21.67 | H | C C |
| | ATOM ATOM | 2058 2059 | N O | GLY H ASN H | 55 56 | 13.904 16.014 | -9.788 -9.067 | 80.282 80.586 | 1.00 25.28 1.00 21.16 | H | |
| | MOTA | 2060 | CA | ASN H | 56 | 16.144 | -9.673 | 81.915 | 1.00 23.73 | H | |
| 05 | ATOM | 2061 | C | ASN H | 56 | 15.330 | -8.806 | 82.892 | 1.00 23.78 | H | C C |
| 65 | ATOM ATOM | 2062 2063 | O CB | ASN H ASN H | 56 56 | 15.336 17.589 | -7.577 -9.632 | 82.747 82.392 | 1.00 27.58 1.00 29.97 | H H | |
| | ATOM | 2064 | CG | ASN H | 56 | 18.530 | -10.453 | 81.518 | 1.00 35.89 | H | |
| | MOTA | 2065 | | ASN H | 56 56 | | -10.418 | 81.706 | 1.00 35.43 | H | _ |
| | ATOM | 2066 | NDZ | ASN H | 56 | 11.9/3 | -11.194 | 80.591 | 1.00 24.91 | H | I N |

| | ATOM | 2067 | N | THR H | 57 | 14.711 | -9.435 | 83.889 | 1.00 19.38 | н | N |
|----|--------------|---------------------|-----------|----------------|--------------------------|------------------|--------------------|------------------|--------------------------|--------|--------------------------|
| | ATOM | 2068 | CA | THR H | 57 | 13.896 | -8.717 | 84.883 | 1.00 16.47 | H | C |
| | ATOM | 2069 | С | THR H | 57 | 14.475 | -8.890 | 86.270 | 1.00 19.01 | H | С |
| | MOTA | 2070 | | THR H | 57 | 15.104 | -9.903 | 86.583 | 1.00 21.14 | H | 0 |
| 5 | MOTA | 2071 | - | THR H | 57 | 12.389 | -9.200 | 84.886 | 1.00 17.39 | H | C |
| | MOTA | 2072 | | THR H | 57 | 12.332 | -10.589 | 85.205 | 1.00 25.30 | H | 0 |
| | MOTA | 2073 | | THR H | 57 | 11.732 | -8.970 | 83.551 | 1.00 16.69 1.00 20.35 | H H | C N |
| | ATOM | 2074 | N | TYR H | 58 50 | 14.232 14.754 | ~7.896 ~7.889 | 87.129 88.475 | 1.00 20.33 | H | G 1/ |
| 40 | ATOM | 2075 | CA | TYR H TYR H | 58 58 | 13.674 | -7.248 | 89.364 | 1.00 17.82 | H | Č |
| 10 | ATOM ATOM | 2076 2077 | C | TYR H | 58 | 13.013 | -6.261 | 88.947 | 1.00 13.98 | H | Ö |
| | ATOM | 2078 | CB | TYR H | 58 | 16.014 | -7.016 | 88.550 | 1.00 16.91 | Н | Č |
| | ATOM | 2079 | CG | TYR H | 58 | 17.033 | -7.287 | 87.445 | 1.00 21.18 | H | C |
| | ATOM | 2080 | | TYR H | 58 | 16.817 | -6.817 | 86.147 | 1.00 20.25 | H | C |
| 15 | ATOM | 2081 | | TYR H | 58 | 18.224 | -7.945 | 87.722 | 1.00 24.53 | H | C |
| | MOTA | 2082 | | TYR H | 58 | 17.759 | -6.965 | 85.163 | 1.00 17.16 | H | Ç |
| | ATOM | 2083 | | TYR H | 58 | 19.180 | -8.128 | 86.727 | 1.00 32.42 | H | C |
| | ATOM | 2084 | CZ | TYR H | 58 | 18.932 | -7.613 | 85.451 84.482 | 1.00 33.73 1.00 41.39 | H H | O C |
| | ATOM | 2085 | OH | TYR H | 58 | 19.898 | -7.689 -7.798 | 90.562 | 1.00 41.39 1.00 17.63 | H | N |
| 20 | ATOM | 2086 2087 | N CA | TYR H TYR H | 59 59 | 13.553 12.533 | -7.347 | 91.504 | 1.00 17.03 | H | Ç |
| | MOTA MOTA | 2088 | CA | TYR H | 59 | 12.996 | -7.474 | 92.932 | 1.00 18.44 | H | č |
| | ATOM | 2089 | ŏ | TYR H | 59 | 13.779 | -8.349 | 93.253 | 1.00 24.99 | H | 0 |
| | ATOM | 2090 | СВ | TYR H | 59 | 11.246 | -8.248 | 91.436 | 1.00 20.01 | H | C |
| 25 | MOTA | 2091 | CG | TYR H | 59 | 10.633 | -8.429 | 90.072 | 1.00 22.20 | H | Č |
| | MOTA | 2092 | CD1 | TYR H | 59 | 10.936 | -9.532 | 89.290 | 1.00 14.53 | H | C |
| | ATOM | 2093 | CD2 | TYR H | 59 | 9.755 | -7.477 | 89.562 88.033 | 1.00 22.20 1.00 14.82 | H | C C |
| | MOTA | 2094 | CE1 | TYR H | 59 59 | 10.389 9.194 | -9.687 -7.616 | 88.314 | 1.00 14.02 | H | č |
| 30 | ATOM ATOM | 2095 2096 | CE2 CZ | TYR H TYR H | 59 59 | 9.528 | -8.736 | 87.549 | 1.00 25.21 | H | č |
| 30 | ATOM | 2097 | OH | TYR H | 59 | 8.996 | -8.828 | 86.300 | 1.00 27.97 | H | O |
| | MOTA | 2098 | N | PRO H | 60 | 12.501 | -6.605 | 93.836 | 1.00 17.68 | Ħ | N |
| | ATOM | 2099 | CA | PRO H | 60 | 12.912 | -6.760 | 95.234 | 1.00 18.52 | H | С |
| | MOTA | 2100 | С | PRO H | 60 | 11.941 | -7.853 | 95.838 | 1.00 23.43 | H | C |
| 35 | MOTA | 2101 | 0 | PRO H | 60 | 10.854 | -8.097 | 95.286 | 1.00 21.98 | H | 0 |
| | MOTA | 2102 | CB | PRO H | 60 | 12.634 | -5.379 | 95.835 95.085 | 1.00 19.08 1.00 17.15 | H H | C C |
| | MOTA | 2103 | CG | PRO H | 60 60 | 11.354 11.714 | -4.978 -5.373 | 93.638 | 1.00 17.13 | H | ç |
| | MOTA MOTA | 2104 2105 | CD N | PRO H ASP H | 61 | 12.307 | -8.462 | 96.962 | 1.00 22.56 | H | Ŋ |
| 40 | ATOM | 2105 | CA | ASP H | 61 | 11.431 | -9.496 | 97.562 | 1.00 23.00 | H | C |
| 70 | ATOM | 2107 | C | ASP H | 61 | 10.045 | -8.987 | 97.911 | 1.00 23.44 | H | С |
| | ATOM | 2108 | 0 | ASP H | 61 | 9.095 | -9.743 | 97.919 | 1.00 26.44 | H | 0 |
| | ATOM | 2109 | CB | ASP H | 61 | 12.083 | | 98.815 | 1.00 22.98 | H | C |
| | MOTA | 2110 | CG | ASP H | 61 | 13.287 | | 98.504 | 1.00 27.24 1.00 27.26 | H H | C |
| 45 | ATOM | 2111 | | ASP H | 61 | 14.042 13.482 | | 99.439 97.327 | 1.00 27.26 1.00 28.00 | п Н | ő |
| | MOTA | 2112 2113 | N N | ASP H SER H | 61 62 | 9.912 | | 98.170 | 1.00 27.64 | H | Ň |
| | MOTA MOTA | $\frac{2113}{2114}$ | CA | SER H | 62 | 8.598 | | 98.526 | 1.00 24.00 | H | C |
| | ATOM | 2115 | C | SER H | 62 | 7.551 | | 97.437 | 1.00 22.42 | H | С |
| 50 | MOTA | 2116 | Õ | SER H | 62 | 6.345 | -7.272 | 97.716 | 1.00 22.71 | H | 0 |
| | MOTA | 2117 | CB | SER H | 62 | 8.751 | | 98.863 | 1.00 22.99 | H | C |
| | ATOM | 2118 | OG | SER H | 62 | 9.242 | | 97.736 | 1.00 22.44 | H | O |
| | MOTA | 2119 | N | VAL H | 63 | 7.967 | | 96.176 95.130 | 1.00 23.61 1.00 26.04 | H H | C N |
| | MOTA | 2120 | CA | VAL H | 63 63 | 6.968 7.147 | | 94.193 | 1.00 20.04 | H | C |
| 55 | ATOM ATOM | $\frac{2121}{2122}$ | C O | VAL H VAL H | 63 | 6.301 | | 93.346 | 1.00 28.27 | H | ŏ |
| | MOTA | 2123 | СВ | VAL H | 63 | 6.819 | | 94.214 | 1.00 25.05 | H | С |
| | ATOM | 2124 | | VAL H | 63 | 6.701 | | 95.086 | 1.00 19.86 | H | С |
| | ATOM | 2125 | | VAL H | 63 | 7.978 | | 93.224 | 1.00 22.12 | H | C |
| 60 | MOTA | 2126 | N | LYS H | 64 | 8.263 | | 94.325 | 1.00 34.01 | H | $\widetilde{\mathbf{N}}$ |
| | MOTA | 2127 | CA | LYS H | 64 | 8.553 | -10.649 | 93.477 | 1.00 37.73 | H | C |
| | ATOM | 2128 | C | LYS H | 64 | | -11.666 | 93.629 | 1.00 36.21 1.00 40.72 | H H | C O |
| | MOTA | 2129 | O | LYS H | 6 <u>4</u> 6 <u>4</u> | 0.985 | -11.943 -11.288 | 94.732 93.897 | 1.00 40.72 | H | C |
| 65 | MOTA | 2130 2131 | CB CG | LYS H LYS H | 64 64 | 10 493 | -12.165 | 92.823 | 1.00 49.69 | H | C |
| 00 | MOTA MOTA | 2132 | CD | LYS H | 64 | 11.595 | -12.977 | 93.447 | 1.00 67.46 | H | Č |
| | MOTA | 2133 | CE | LYS H | 64 | 12.336 | -13.781 | 92.388 | 1.00 84.78 | H | С |
| | ATOM | 2134 | NZ | LYS H | 64 | 12.931 | 15.014 | 93.018 | 1.00 92.94 | H | N |
| | MOTA | 2135 | N | GLY H | 65 | 6.967 | -12.177 | 92.504 | 1.00 34.99 | H | N |
| | | | | | | | | | | | |

| | - TIOM | 2126 | 07 OT 37 | 11 6 | 55 | 5 07 <i>6</i> | -13.134 | 92,522 | 1.00 33.39 | Н | ı c |
|-----|--------------|----------------|----------|------|----------|-----------------|------------------|------------------|--------------------------|--------|-----|
| | ATOM ATOM | 2136 2137 | CA GLY | | 55 | | -12.447 | 92.308 | 1.00 33.65 | H | |
| | ATOM | 2138 | O GLY | | 55 | | -13.076 | 91.859 | 1.00 40.69 | Н | |
| | ATOM | 2139 | N ARG | | 6 | 4.471 | -11.147 | 92.609 | 1.00 29.54 | H | |
| 5 | MOTA | 2140 | CA ARG | н 6 | 6 | 3.222 | -10.420 | 92.455 | 1.00 23.99 | Н | |
| | MOTA | 2141 | C ARG | _ | 6 | 3.205 | -9.377 | 91.343 | 1.00 27.36 | H | |
| | ATOM | 2142 | O ARG | | 6 | 2.144 | -9.079 -9.740 | 90.802 93.767 | 1.00 26.62 1.00 24.49 | H H | |
| | ATOM | 2143 | CB ARG | | 66 66 | 2.872 2.673 | -10.671 | 94.956 | 1.00 24.49 | H | |
| 10 | ATOM ATOM | $2144 \\ 2145$ | CG ARG | _ | 56 | 2.156 | -9.875 | 96.177 | 1.00 26.28 | H | |
| 10 | ATOM | 2145 | NE ARG | | 56 | 3.013 | -8.738 | 96.549 | 1.00 26.58 | H | |
| | ATOM | 2147 | CZ ARG | | 56 | 2.590 | -7.468 | 96.631 | 1.00 23.28 | H | C C |
| | ATOM | 2148 | NH1 ARG | | 56 | 1.325 | -7.156 | 96.356 | 1.00 20.50 | H | |
| | MOTA | 2149 | NH2 ARG | | 56 | 3.429 | -6.513 | 97.026 | 1.00 23.33 | H | |
| 15 | ATOM | 2150 | N PHE | | 57 | 4.377 | -8.805 | 91.041 | 1.00 28.25 1.00 28.94 | H | |
| | ATOM | 2151 | CA PHE | | 57 | 4.527 5.356 | -7.775 -8.293 | 90.002 88.845 | 1.00 28.94 | H H | |
| | MOTA MOTA | 2152 2153 | C PHE | | 57 57 | 6.344 | -8.982 | 89.047 | 1.00 28.35 | H | |
| | ATOM | 2154 | CB PHE | | 57 57 | 5.291 | -6.533 | 90.563 | 1.00 32.76 | . Н | |
| 20 | MOTA | 2155 | CG PHE | | 57 | 4.496 | -5.690 | 91.510 | 1.00 35.90 | H | ı C |
| | MOTA | 2156 | CD1 PHE | | 57 | 3.336 | -6.190 | 92.108 | 1.00 32.82 | H | |
| | ATOM | 2157 | CD2 PHE | | 57 | 4.934 | -4.407 | 91.843 | 1.00 27.67 | H | |
| | MOTA | 2158 | CE1 PHE | | 57 | 2.620 | -5.421 | 93.032 92.758 | 1.00 37.74 1.00 34.67 | H. | |
| 0.5 | MOTA | 2159 | CE2 PHE | | 57 57 | 4.236 3.081 | -3.644 -4.138 | 93.358 | 1.00 34.67 | H | |
| 25 | MOTA MOTA | 2160 2161 | N THE | | 58 | 4.962 | -7.937 | 87.637 | 1.00 28.82 | F | |
| | MOTA | 2162 | CA THE | | 68 | 5.726 | -8.301 | 86.457 | 1.00 29.24 | H | ı C |
| | MOTA | 2163 | C THE | ιн 6 | 58 | 5.964 | -7.073 | 85.574 | 1.00 28.81 | F | |
| | MOTA | 2164 | O THE | | 68 | 5.009 | -6.399 | 85.175 | 1.00 29.95 | H | |
| 30 | ATOM | 2165 | CB THE | | 68 | 4.940 | -9.382 | 85.611 86.463 | 1.00 31.63 1.00 28.51 | F F | |
| | ATOM | 2166 2167 | OG1 THE | | 68 68 | 4.660 5.735 | -10.484 -9.824 | 84.396 | 1.00 23.31 | ŀ | |
| | ATOM ATOM | 2168 | N ILE | | 69 | 7.227 | -6.779 | 85.268 | 1.00 24.66 | F | |
| | MOTA | 2169 | CA ILE | | 69 | 7.546 | -5.666 | 84.369 | 1.00 25.58 | F | |
| 35 | MOTA | 2170 | C ILE | | 69 | 7.756 | -6.235 | 82.965 | 1.00 27.22 | H | |
| | MOTA | 2171 | O ILF | | 69 | 8.245 | | 82.839 | 1.00 31.09 | | 0 I |
| | MOTA | 2172 | CB ILI | | 69 | 8.852 | -4.947 | 84.841 | 1.00 26.43 | ŀ | |
| | MOTA | 2173 | CG1 ILE | | 69 69 | 9.127 10.060 | -3.732 -5.907 | 83.959 84.829 | 1.00 18.67 1.00 28.93 | F | H C |
| 40 | MOTA MOTA | 2174 2175 | CG2 ILE | | 69 | 10.299 | | 84.578 | 1.00 22.12 | | i C |
| 40 | ATOM | 2176 | N SEI | | 70 | 7.369 | | 81.924 | 1.00 24.59 | | H N |
| | ATOM | 2177 | CA SEI | | 70 | 7.542 | -5.962 | 80.560 | 1.00 20.35 | | H C |
| | MOTA | 2178 | C SE | | 70 | 7.651 | | 79.670 | 1.00 20.76 | | H C |
| | ATOM | 2179 | O SEI | | 70 | 7.380 | | 80.110 | 1.00 22.20 1.00 18.01 | | H C |
| 45 | MOTA | 2180 2181 | CB SEI | | 70 70 | 6.326 5.148 | | 80.156 80.171 | 1.00 18.01 | | H O |
| | MOTA MOTA | 2181 | OG SEI | | 70 71 | 8.080 | | 78.430 | 1.00 21.74 | | H N |
| | ATOM | 2183 | CA ARC | | 71 | 8.197 | | 77.546 | 1.00 22.80 | F | H C |
| | MOTA | 2184 | C ARC | | 71 | 7.718 | -4.155 | 76.155 | 1.00 25.05 | | H C |
| 50 | MOTA | 2185 | | | 71 | 7.855 | | 75.693 | 1.00 28.88 | | O E |
| | ATOM | 2186 | CB ARG | | 71 | 9.679 | | 77.440 | 1.00 22.32 1.00 17.63 | | H C |
| | ATOM | 2187 | | | 71 71 | 10.654 12.132 | | 76.878 77.230 | 1.00 17.83 | | H C |
| | MOTA MOTA | 2188 2189 | _ | | 71 | 12.522 | | 76.577 | 1.00 26.63 | | H N |
| 55 | ATOM | 2190 | | | 71 | 13.529 | | 76.974 | 1.00 20.51 | | H C |
| ••• | ATOM | 2191 | NH1 ARG | | 71 | 14.253 | -2.413 | 78.030 | 1.00 13.73 | | H N |
| | MOTA | 2192 | NH2 AR | 3 Н | 71 | 13.792 | | 76.324 | 1.00 17.61 | | H N |
| | MOTA | 2193 | | | 72 | 7.190 | | 75.464 | 1.00 24.41 | | H N |
| 00 | MOTA | 2194 | | | 72 73 | 6.788 | | 74.094 73.272 | 1.00 24.18 1.00 25.45 | | H C |
| 60 | MOTA MOTA | 2195 2196 | | | 72 72 | 7.709 7.498 | | 73.272 | 1.00 25.45 | | H O |
| | ATOM | 2196 | | | 72 | 5.333 | | 73.865 | 1.00 27.17 | | H Č |
| 131 | MOTA | 2198 | | | 72 | 4.914 | -3.198 | 72.416 | 1.00 30.78 | 1 | H C |
| | MOTA | 2199 | OD1 AS | РН | 72 | 5.759 | -2.993 | 71.510 | 1.00 33.98 | | H O |
| 65 | MOTA | 2200 | OD2 AS | | 72 | 3.741 | | 72.194 | 1.00 38.58 | | H O |
| | ATOM | 2201 | | | 73 | 8.752 | | 72.711 71.912 | 1.00 26.35 1.00 29.04 | | H C |
| | MOTA | 2202 2203 | | | 73 73 | 9.720 9.235 | | 70.569 | 1.00 29.04 | | H C |
| | MOTA MOTA | 2204 | | | 73 73 | 9.895 | | 69.945 | 1.00 28.40 | | H O |
| | | | | | | | | | | | |

| | ATOM | 2205 | CB | ASN H | 73 | 10.958 | -3.246 | 71.675 | 1.00 31.88 | | ** | ~ |
|-----|-------|------|--------------|---------|----|--------|--------|--------|------------|---|----|---|
| | ATOM | 2206 | | | | 11.812 | -3.396 | | | | H | C |
| | ATOM | 2207 | | 1 ASN H | | | | | 1.00 32.53 | | H | C |
| | | | | | | 11.632 | -2.669 | 73.912 | 1.00 42.74 | | H | 0 |
| _ | ATOM | 2208 | | 2 ASN H | | 12.759 | -4.319 | 72.877 | 1.00 33,41 | | H | N |
| 5 | MOTA | 2209 | N | ALA H | 74 | 8.076 | -2.276 | 70.115 | 1.00 32.65 | | H | |
| | ATOM | 2210 | CA | ALA H | 74 | 7.595 | -1.739 | | | | | N |
| | MOTA | 2211 | C | ALA H | | 6.852 | | | 1.00 32.57 | | H | C |
| | ATOM | 2212 | | | | | -0.422 | 69.164 | 1.00 33.69 | | H | C |
| | | | 0 | ALA H | | 6.922 | 0.547 | 68.421 | 1.00 31.16 | | H | 0 |
| | MOTA | 2213 | CB | ALA H | 74 | 6.660 | -2.771 | 68.187 | 1.00 29.62 | | H | Č |
| 10 | ATOM | 2214 | N | ARG H | 75 | 6.189 | -0.399 | 70.311 | 1.00 32.12 | | | |
| | MOTA | 2215 | CA | ARG H | | 5.408 | 0.758 | | | | H | N |
| | MOTA | 2216 | C | ARG H | | | | 70.729 | 1.00 32.75 | | H | C |
| | | | | | | 6.097 | 1.695 | 71.737 | 1.00 29.96 | | H | C |
| | ATOM | 2217 | 0 | ARG H | | 5.565 | 2.771 | 72.030 | 1.00 28.48 | | H | Ō |
| | ATOM | 2218 | CB | ARG H | 75 | 4.071 | 0.276 | 71.327 | 1.00 35.04 | | H | |
| 15 | ATOM | 2219 | CG | ARG H | 75 | 3.111 | -0.412 | 70.334 | | | | C |
| | MOTA | 2220 | CD | ARG H | 75 | 1.825 | | | 1.00 40.61 | | H | C |
| | ATOM | | | | | | -0.875 | 71.046 | 1.00 61.45 | | H | C |
| | | 2221 | NE | ARG H | 75 | 0.853 | -1.612 | 70.224 | 1.00 68.33 | | H | N |
| | MOTA | 2222 | CZ | ARG H | 75 | 1.029 | -2.841 | 69.731 | 1.00 69.94 | | Н | Ċ |
| | ATOM | 2223 | NH: | L ARG H | 75 | 2.157 | -3.513 | 69.950 | 1.00 60.61 | | | |
| 20 | ATOM | 2224 | MHO | ARG H | 75 | 0.045 | -3.419 | | | | H | N |
| | ATOM | 2225 | N | | | | | 69.040 | 1.00 70.68 | | H | N |
| | | | | ASN H | 76 | 7.271 | 1.307 | 72.249 | 1.00 27.39 | | H | N |
| | ATOM | 2226 | CA | ASN H | 76 | 7.995 | 2.149 | 73.236 | 1.00 22.45 | | H | С |
| | MOTA | 2227 | C | ASN H | 76 | 7.114 | 2.344 | 74.461 | 1.00 24.26 | | H | Č |
| | ATOM | 2228 | 0 | ASN H | 76 | 6.883 | 3.462 | 74.915 | 1.00 27.85 | | | |
| 25 | ATOM | 2229 | CB | ASN H | 76 | 8.347 | 3.546 | | | | H | 0 |
| | ATOM | 2230 | | | | | | 72.680 | 1.00 22.88 | | H | C |
| | | | CG | ASN H | 76 | 9.606 | 3.558 | 71.780 | 1.00 30.19 | | H | С |
| | ATOM | 2231 | | ASN H | 76 | 10.162 | 4.622 | 71.501 | 1.00 45.69 | | H | 0 |
| | ATOM | 2232 | ND2 | ASN H | 76 | 10.045 | 2.411 | 71.354 | 1.00 27.13 | | H | N |
| | MOTA | 2233 | N | ILE H | 77 | 6.624 | 1.251 | 75.001 | | | | |
| 30 | MOTA | 2234 | ĈA | ILE H | 77 | | | | 1.00 20.55 | | H | N |
| | ATOM | | | | | 5.783 | 1.289 | 76.166 | 1.00 21.43 | | H | C |
| | | 2235 | C | ILE H | 77 | 6.347 | 0.293 | 77.178 | 1.00 26.35 | | H | С |
| | ATOM | 2236 | 0 | ILE H | 77 | 6.750 | -0.825 | 76.833 | 1.00 27.67 | | H | ō |
| | ATOM | 2237 | CB | ILE H | 77 | 4.314 | 0.848 | 75.819 | 1.00 25.31 | | | |
| | MOTA | 2238 | CG1 | | 77 | 3.752 | 1.702 | | | | H | C |
| 35 | ATOM | 2239 | CG2 | | | | | 74.674 | 1.00 31.02 | | H | С |
| 00 | | | | | 77 | 3.455 | 0.930 | 77.069 | 1.00 24.50 | | H | C |
| | MOTA | 2240 | CDI | . ILE H | 77 | 2.332 | 1.304 | 74.167 | 1.00 18.41 | | H | С |
| | ATOM | 2241 | \mathbf{N} | LEU H | 78 | 6.381 | 0.703 | 78.436 | 1.00 27.91 | | H | N |
| | MOTA | 2242 | CA | LEU H | 78 | 6.874 | -0.106 | 79.528 | | | | |
| | ATOM | 2243 | Č | LEU H | 78 | | | | 1.00 24.89 | | H | С |
| 40 | ATOM | 2244 | | | | 5.645 | -0.396 | 80.365 | 1.00 24.76 | | H | C |
| 40 | | | 0 | LEU H | 78 | 4.866 | 0.506 | 80.598 | 1.00 25.50 | | H | 0 |
| | MOTA | 2245 | CB | LEU H | 78 | 7.851 | 0.727 | 80.405 | 1.00 24.49 | | H | C |
| | ATOM | 2246 | CG | LEU H | 78 | 8.376 | 0.043 | 81.650 | 1.00 18.05 | | H | Č |
| | MOTA | 2247 | CD1 | LEU H | 78 | 9.449 | -1.026 | 81.241 | 1.00 27.00 | | | |
| | ATOM | 2248 | | LEU H | 78 | 9.068 | | | | | H | С |
| 45 | ATOM | 2249 | | TYR H | | | 1.102 | 82.532 | 1.00 15.70 | | H | C |
| 40 | | | N | | 79 | 5.484 | -1.630 | 80.833 | 1.00 26.11 | | H | N |
| | ATOM | 2250 | CA | TYR H | 79 | 4.330 | -1.997 | 81.662 | 1.00 25.62 | | H | C |
| | MOTA | 2251 | C | TYR H | 79 | 4.720 | -2.514 | 83.014 | 1.00 27.75 | | H | č |
| | ATOM | 2252 | 0 | TYR H | 79 | 5.827 | -3.036 | 83.193 | 1.00 29.83 | | | |
| | ATOM | 2253 | CB | TYR H | 79 | 3.525 | | | 1.00 29.83 | | H | 0 |
| 50 | ATOM | 2254 | | | | | -3.156 | 80.994 | 1.00 22.60 | | H | С |
| 00 | | | CG | TYR H | 79 | 2.952 | -2.791 | 79.652 | 1.00 27.08 | | H | С |
| | ATOM | 2255 | | TYR H | 79 | 3.565 | -3.195 | 78.479 | 1.00 20.92 | | H | C |
| | MOTA | 2256 | CD2 | TYR H | 79 | 1.791 | -2.020 | 79.556 | 1.00 24.64 | | H | Č |
| | ATOM | 2257 | | TYR H | 79 | 3.048 | -2.848 | 77.247 | | | | ~ |
| | ATOM | 2258 | CES | TYR H | 79 | | | | 1.00 24.71 | | H | C |
| 55 | ATOM | | | | | 1.277 | -1.668 | 78.323 | 1.00 21.72 | | H | C |
| 33 | | 2259 | CZ | TYR H | 79 | 1.908 | -2.084 | 77.173 | 1.00 24.82 | | H | С |
| | ATOM | 2260 | OH | TYR H | 79 | 1.423 | -1.711 | 75.935 | 1.00 21.43 | | H | ō |
| | ATOM | 2261 | N | LEU H | 80 | 3.779 | -2.429 | 83.964 | 1.00 25.48 | | | |
| | ATOM | 2262 | CA | LEU H | 80 | 3.947 | -3.007 | 05.204 | | | H | N |
| | MOTA | 2263 | C | LEU H | | | | 85.272 | 1.00 25.75 | | H | C |
| 60 | | | | | 80 | 2.592 | -3.669 | 85.596 | 1.00 27.57 | | H | С |
| 00 | ATOM | 2264 | 0 | LEU H | 80 | 1.599 | -2.983 | 85.835 | 1.00 34.28 | | H | 0 |
| | MOTA | 2265 | CB | LEU H | 80 | 4.245 | -1.992 | 86.409 | 1.00 25.22 | | H | Č |
| | ATOM | 2266 | CG | LEU H | 80 | 4.468 | -2.735 | 87.754 | 1.00 25.22 | | | |
| | MOTA | 2267 | | LEU H | 80 | | | | | | H | С |
| | | | | | | 5.836 | -3.504 | 87.721 | 1.00 18.29 | | H | C |
| e E | ATOM | 2268 | | LEU H | 80 | 4.552 | -1.721 | 88.992 | 1.00 20.69 | | H | C |
| 65 | MOTA | 2269 | N | GLN H | 81 | 2.550 | -4.993 | 85.563 | 1.00 30.10 | | H | N |
| | MOTA | 2270 | CA | GLN H | 81 | 1.318 | -5.716 | 85.905 | 1.00 32.07 | | H | |
| | MOTA | 2271 | C | GLN H | 81 | 1.409 | -6.033 | 87.376 | | | | C |
| | MOTA | 2272 | ŏ | GLN H | 81 | | | | 1.00 30.52 | | H | C |
| | ATOM | 2273 | | | | 2.379 | -6.674 | 87.832 | 1.00 30.77 |] | H | 0 |
| | TI OH | 4413 | CB | GLN H | 81 | 1.224 | -7.029 | 85.104 | 1.00 34.27 |] | H | С |
| | | | | | | | | | | | | |

| | ATOM | 2274 | CG GLN H | 81 | 0.084 | -7.955 | 85.580 | 1.00 36.03 | Н | С |
|-----|--------------|--------------|------------------------|------------|------------------|------------------|------------------|--------------------------|--------|---------|
| | MOTA | 2275 | CD GLN H | 81 | -1.266 | -7.341 | 85.316 | 1.00 40.10 | H | C |
| | ATOM | 2276 | OE1 GLN H | 81 | -2.047 | -7.096 | 86.248 | 1.00 35.51 | H | 0 |
| - | ATOM | 2277 | NE2 GLN H | 81 | -1.543 0.428 | -7.047 -5.573 | 84.053 88.153 | 1.00 29.75 1.00 29.32 | H H | N N |
| 5 | MOTA MOTA | 2278 2279 | N MET H CA MET H | 82 82 | 0.426 | | 89.579 | 1.00 23.52 | H | Č |
| | ATOM | 2279 | C MET H | 82 | -0.719 | | 89.911 | 1.00 33.42 | H | Č |
| | ATOM | 2281 | O MET H | 82 | -1.784 | | 89.386 | 1.00 37.22 | H | ō |
| | ATOM | 2282 | CB MET H | 82 | 0.305 | -4.526 | 90.380 | 1.00 32.57 | H | С |
| 10 | ATOM | 2283 | CG MET H | 82 | 1.424 | -3.501 | 90.097 | 1.00 34.83 | H | C |
| | MOTA | 2284 | SD MET H | 82 | 1.236 | | 91.036 | 1.00 41.35 | H | S |
| | MOTA | 2285 | CE MET H | 82 | 0.076 | | 90.153 | 1.00 21.34 | H | C |
| | MOTA | 2286 | N SER H | 82A | -0.500 | | 90.789 | 1.00 33.87 | H | N |
| | ATOM | 2287 | CA SER H | 82A | -1.553 | | 91.161 92.664 | 1.00 32.69 1.00 30.35 | H H | C |
| 15 | ATOM | 2288 2289 | C SER H O SER H | 82A 82A | -1.455 -0.448 | | 93.253 | 1.00 30.33 | H | Ö |
| | MOTA MOTA | 2290 | CB SER H | 82A | -1.309 | | 90.445 | 1.00 30.90 | H | č |
| | ATOM | 2291 | OG SER H | 82A | -0.074 | | 90.886 | 1.00 39.97 | H | Ō |
| | ATOM | 2292 | N SER H | 82B | -2.456 | | 93.270 | 1.00 30.11 | H | N |
| 20 | MOTA | 2293 | CA SER H | 82B | -2.532 | | 94.738 | 1.00 32.59 | H | С |
| | MOTA | 2294 | C SER H | 82B | -2.084 | | 95.464 | 1.00 34.41 | H | Ċ |
| | ATOM | 2295 | O SER H | 82B | -1.256 | | 96.386 | 1.00 34.38 | H | 0 |
| | MOTA | 2296 | CB SER H | 82B | -1.670 | | 95.249 94.545 | 1.00 31.62 1.00 39.73 | H H | C O |
| 05 | MOTA | 2297 | OG SER H | 82B 82C | -1.941 -2.646 | | 95.050 | 1.00 34.50 | H | N |
| 25 | MOTA MOTA | 2298 2299 | N LEU H | 82C | -2.300 | | 95.687 | 1.00 34.52 | H | Č |
| | ATOM | 2300 | C FER H | 82C | -2.677 | | 97.154 | 1.00 33.77 | н | Ċ |
| | ATOM | 2301 | O LEU H | 82C | -3.731 | | 97.563 | 1.00 36.50 | H | 0 |
| | ATOM | 2302 | CB LEU H | 82C | -2.965 | -4.745 | 94.923 | 1.00 31.33 | H | С |
| 30 | ATOM | 2303 | CG LEU H | 82C | -2.300 | | 93.556 | 1.00 29.69 | H | C |
| | MOTA | 2304 | CD1 LEU H | 82C | -3.142 | | 92.586 | 1.00 14.81 | H | C |
| | ATOM | 2305 | CD2 LEU H | 82C | -0.928 | | | 1.00 22.96 1.00 37.50 | H H | C N |
| | ATOM | 2306 | N ARG H | 83 83 | -1.794 -1.967 | | 97.953 99.404 | 1.00 37.30 | п Н | C |
| 35 | MOTA MOTA | 2307 2308 | CA ARG H C ARG H | 83 | -2.044 | | | 1.00 37.20 | H | č |
| 35 | MOTA | 2309 | O ARG H | 83 | -1.641 | | | 1.00 34.41 | H | õ |
| | ATOM | 2310 | CB ARG H | 83 | -0.753 | | 100.115 | 1.00 35.83 | H | C |
| | MOTA | 2311 | CG ARG H | 83 | -0.474 | -7.134 | 99.749 | 1.00 44.13 | H | С |
| | MOTA | 2312 | CD ARG H | 83 | 0.963 | | 100.035 | 1.00 58.61 | H | С |
| 40 | MOTA | 2313 | NE ARG H | 83 | 1.255 | | | 1.00 65.92 | H | N |
| | MOTA | 2314 | CZ ARG H | 83 | 2.452 | | | 1.00 68.29 1.00 66.48 | H H | N C |
| | MOTA | 2315 | NH1 ARG H NH2 ARG H | 83 83 | 3.467 2.628 | | 100.328 | 1.00 76.67 | H | N |
| | ATOM ATOM | 2316 2317 | NH2 ARG H N SER H | 84 | -2.518 | | 100.887 | 1.00 33.54 | H | N |
| 45 | MOTA | 2318 | CA SER H | 84 | -2.634 | | 101.209 | 1.00 31.43 | H | C |
| -10 | ATOM | 2319 | C SER H | 84 | -1.268 | | 101.096 | 1.00 30.46 | H | C |
| | ATOM | 2320 | O SER H | 84 | -1.188 | | 100.617 | 1.00 27.90 | H | 0 |
| | ATOM | 2321 | CB SER H | 84 | -3.223 | | 102.606 | 1.00 32.69 | H | C |
| | MOTA | 2322 | OG SER H | 84 | -2.303 | | 103.617 | 1.00 45.64 | H | O NT |
| 50 | ATOM | 2323 | N GLU H | 85 | -0.218 1.174 | | 101.491 | 1.00 27.55 1.00 28.67 | H H | C N |
| | ATOM ATOM | 2324 2325 | CA GLU H C GLU H | 85 85 | 1.693 | | 100.071 | 1.00 27.89 | H | Č |
| | ATOM | 2326 | O GLU H | 85 | 2.72 | | | 1.00 31.91 | H | ŏ |
| | MOTA | 2327 | CB GLU H | 85 | 2.15 | 3 -2.463 | 102.036 | 1.00 28.80 | H | C |
| 55 | ATOM | 2328 | CG GLU H | 85 | 1.71 | -3.123 | 103.296 | 1.00 46.74 | H | C |
| | MOTA | 2329 | CD GLU H | 85 | 0.84 | 4 -4.321 | 103.003 | 1.00 56.38 | Н | C |
| | MOTA | 2330 | OE1 GLU H | 85 | 1.39 | | 102.632 | 1.00 62.51 | H | 0 |
| | MOTA | 2331 | OE2 GLU H | 85 | -0.38 | | 103.105 | 1.00 56.24 | H | 0 |
| 00 | ATOM | 2332 | N ASP H | 86 | 1.03 | | | 1.00 25.29 1.00 25.71 | H H | C N |
| 60 | MOTA | 2333 | CA ASP H | 86 86 | 1.429 | | | 1.00 25.71 | H | Ç |
| | ATOM ATOM | 2334 2335 | C ASP H O ASP H | 86 86 | 1.07 | | 96.147 | 1.00 25.68 | H | ŏ |
| | ATOM | 2336 | CB ASP H | 86 | 0.90 | | | 1.00 26.58 | H | Č |
| | MOTA | 2337 | CG ASP H | 86 | 1.41 | | 96.877 | 1.00 32.52 | H | C |
| 65 | MOTA | 2338 | OD1 ASP H | 86 | 0.58 | 6 -4.562 | 96.763 | 1.00 30.42 | H | 0 |
| | MOTA | 2339 | OD2 ASP H | 86 | 2.62 | | | 1.00 29.99 | H | 0 |
| | MOTA | 2340 | N THR H | 87 | 0.07 | | | 1.00 23.93 | H | N |
| | MOTA | 2341 | CA THR H | 87 87 | -0.53 | | | 1.00 23.44 1.00 22.23 | H H | C C |
| | ATOM | 2342 | C THR H | 87 | 0.66 | 1 3.163 | 0 91.090 | 1.00 44.43 | п | C |

| | MOTA | 2343 | 0 | THR H | 87 | 1.447 | 3.314 | 98.591 | 1.00 21.36 | H | 0 1 |
|------|-------|------|-------------|-------|-----|--------|--------|--------|------------|---|-----|
| | ATOM | 2344 | CB | THR H | 87 | -1.458 | 2.654 | 98.956 | 1.00 26.73 | H | |
| | ATOM | 2345 | OG1 | | 87 | -2.623 | 1.808 | 98.992 | 1.00 26.03 | | - |
| | ATOM | 2346 | CG2 | | 87 | -1.881 | | | | H | |
| 5 | MOTA | | | | | | 4.145 | 98.709 | 1.00 28.47 | H | |
| 3 | | 2347 | N | ALA H | 88 | 0.722 | 3.845 | 96.568 | 1.00 19.07 | H | I N |
| | ATOM | 2348 | ca | ALA H | 88. | 1.889 | 4.717 | 96.354 | 1.00 17.45 | H | |
| | MOTA | 2349 | C | ALA H | 88 | 1.815 | 5.404 | 95.052 | 1.00 21.75 | H | |
| | ATOM | 2350 | 0 | ALA H | 88 | 0.972 | 5.103 | 94.182 | 1.00 21.21 | H | |
| | ATOM | 2351 | ČВ | ALA H | 88 | 3.162 | | | | | |
| 10 | | | | | | | 3.843 | 96.361 | 1.00 14.94 | H | C |
| 10 | ATOM | 2352 | N | MET H | 89 | 2.746 | 6.358 | 94.868 | 1.00 22.41 | H | I N |
| | ATOM | 2353 | $^{\rm CA}$ | MET H | 89 | 2.827 | 7.001 | 93.570 | 1.00 24.72 | н | |
| | ATOM | 2354 | С | MET H | 89 | 3.794 | 6.092 | 92.835 | 1.00 22.60 | н | |
| | ATOM | 2355 | Ō | MET H | 89 | 4.839 | 5.790 | 93.399 | 1.00 26.75 | | |
| | MOTA | 2356 | ČВ | MET H | 89 | | | | | H | |
| 4 == | | | | | | 3.516 | 8.378 | 93.679 | 1.00 24.18 | H | |
| 15 | ATOM | 2357 | CG | MET H | 89 | 3.623 | 9.117 | 92.352 | 1.00 24.57 | H | C |
| | MOTA | 2358 | SD | MET H | 89 | 2.092 | 9.565 | 91.500 | 1.00 31.14 | H | |
| | ATOM | 2359 | $^{\rm CE}$ | MET H | 89 | 1.586 | 10.985 | 92.556 | 1.00 17.32 | H | |
| | MOTA | 2360 | N | TYR H | 90 | 3.478 | 5.699 | 91.598 | 1.00 19.66 | | |
| | MOTA | 2361 | ĈA | TYR H | 90 | | | | | H | |
| 20 | | | | | | 4.390 | 4.838 | 90.830 | 1.00 18.76 | H | |
| 20 | ATOM | 2362 | C | TYR H | 90 | 5.026 | 5.618 | 89.717 | 1.00 19.48 | H | C |
| | ATOM | 2363 | 0 | TYR H | 90 | 4.343 | 6.131 | 88.836 | 1.00 18.22 | Н | |
| | ATOM | 2364 | CB | TYR H | 90 | 3.643 | 3.600 | 90.214 | 1.00 16.54 | Н | |
| | MOTA | 2365 | CG | TYR H | 90 | 3.375 | 2.566 | 91.286 | 1.00 14.14 | H | |
| | ATOM | 2366 | | TYR H | 90 | 4.172 | | | | | |
| 25 | | | | | | | 1.427 | 91.392 | 1.00 9.33 | H | |
| 25 | MOTA | 2367 | | TYR H | 90 | 2.376 | 2.772 | 92.251 | 1.00 22.63 | H | С |
| | ATOM | 2368 | CE1 | | 90 | 3.988 | 0.522 | 92.425 | 1.00 15.98 | H | C |
| | MOTA | 2369 | CE2 | TYR H | 90 | 2.197 | 1.887 | 93.285 | 1.00 13.30 | Н | |
| | ATOM | 2370 | CZ | TYR H | 90 | 3.009 | 0.760 | 93.361 | 1.00 24.24 | H | |
| | ATOM | 2371 | OH | TYR H | 90 | 2.835 | -0.114 | 94.384 | | | |
| 30 | MOTA | | | | | | | | 1.00 21.02 | H | |
| 30 | | 2372 | N | TYR H | 91 | 6.368 | 5.669 | 89.721 | 1.00 20.31 | H | N |
| | ATOM | 2373 | CA | TYR H | 91 | 7.094 | 6.384 | 88.651 | 1.00 17.12 | H | С |
| | MOTA | 2374 | С | TYR H | 91 | 7.769 | 5.400 | 87.681 | 1.00 19.92 | Н | |
| | ATOM | 2375 | 0 | TYR H | 91 | 8.393 | 4.441 | 88.121 | 1.00 18.18 | | |
| | ATOM | 2376 | ČВ | TYR H | | | | | | H | |
| 05 | | | | | 91 | 8.251 | 7.216 | 89.226 | 1.00 15.44 | H | |
| 35 | ATOM | 2377 | CG | TYR H | 91 | 7.793 | 8.338 | 90.138 | 1.00 17.08 | H | С |
| | MOTA | 2378 | CD1 | TYR H | 91 | 7.818 | 8.208 | 91.507 | 1.00 9.66 | H | |
| | ATOM | 2379 | CD2 | TYR H | 91 | 7.339 | 9.525 | 89.589 | 1.00 15.29 | H | _ |
| | ATOM | 2380 | CE1 | | 91 | 7.408 | 9.260 | 92.338 | 1.00 16.34 | | č |
| | MOTA | 2381 | CE2 | | | | | | | H | |
| 40 | | | | | 91 | 6.901 | 10.577 | 90.398 | 1.00 15.56 | H | С |
| 40 | ATOM | 2382 | CZ | TYR H | 91 | 6.944 | 10.446 | 91.755 | 1.00 21.42 | H | С |
| | MOTA | 2383 | OH | TYR H | 91 | 6.544 | 11.517 | 92.547 | 1.00 8.81 | H | |
| | ATOM | 2384 | N | CYS H | 92 | 7.650 | 5.733 | 86.397 | 1.00 21.55 | H | |
| | MOTA | 2385 | CA | CYS H | 92 | 8.311 | 5.065 | 85.278 | 1.00 21.33 | | |
| | ATOM | 2386 | | | | | | | | H | |
| 45 | | | C | CYS H | 92 | 9.709 | 5.751 | 85.270 | 1.00 20.94 | H | |
| 45 | MOTA | 2387 | 0 | CYS H | 92 | 9.771 | 6.959 | 85.435 | 1.00 20.43 | H | 0 |
| | MOTA | 2388 | CB | CYS H | 92 | 7.602 | 5.498 | 83.987 | 1.00 18.81 | H | |
| | MOTA | 2389 | SG | CYS H | 92 | 8.429 | 4.801 | 82.569 | 1.00 32.60 | H | |
| | MOTA | 2390 | N | ALA H | 93 | 10.805 | 5.022 | 85.095 | 1.00 18.52 | | |
| | ATOM | 2391 | CA | ALA H | | | | | | H | N |
| EO | | | | | 93 | 12.107 | 5.684 | 85.085 | 1.00 15.79 | H | C |
| 50 | ATOM | 2392 | C | ALA H | 93 | 13.066 | 5.019 | 84.068 | 1.00 15.40 | H | C |
| | ATOM | 2393 | 0 | ALA H | 93 | 13.031 | 3.780 | 83.898 | 1.00 20.16 | H | |
| | MOTA | 2394 | CB | ALA H | 93 | 12.737 | 5.604 | 86.462 | 1.00 16.78 | H | č |
| | ATOM | 2395 | N | ARG H | 94 | 13.898 | 5.821 | 83.402 | | | |
| | ATOM | 2396 | CA | | | | | | 1.00 15.89 | H | N |
| EE | | | | ARG H | 94 | 14.873 | 5.224 | 82.480 | 1.00 17.43 | H | С |
| 55 | ATOM | 2397 | C | ARG H | 94 | 16.031 | 4.849 | 83.374 | 1.00 17.10 | H | C |
| | MOTA | 2398 | 0 | ARG H | 94 | 16.607 | 5.705 | 84.058 | 1.00 16.11 | H | 0 |
| | MOTA | 2399 | CB | ARG H | 94 | 15.325 | 6.211 | 81.417 | 1.00 13.45 | H | č |
| | ATOM | 2400 | CG | ARG H | 94 | 16.050 | 5.523 | 00 330 | | | Č |
| | | | | | | | | 80.238 | 1.00 15.86 | H | C |
| 00 | ATOM | 2401 | CD | ARG H | 94 | 16.477 | 6.566 | 79.242 | 1.00 13.79 | H | C |
| 60 | ATOM | 2402 | NE | ARG H | 94 | 17.730 | 7.229 | 79.580 | 1.00 17.29 | H | N |
| | ATOM | 2403 | CZ | ARG H | 94 | 18.301 | 8.146 | 78.818 | 1.00 20.35 | H | Ċ |
| | ATOM | 2404 | | ARG H | 94 | 17.705 | 8.549 | 77.664 | 1.00 13.04 | | |
| | ATOM | 2405 | | ARG H | 94 | | | | | H | N |
| | | | | | | 19.520 | 8.602 | 79.142 | 1.00 15.82 | H | N |
| 05 | ATOM | 2406 | N | LEU H | 95 | 16.397 | 3.565 | 83.350 | 1.00 19.09 | H | N |
| 65 | MOTA | 2407 | CA | LEU H | 95 | 17.469 | 3.079 | 84.217 | 1.00 17.64 | H | C |
| | ATOM | 2408 | C | LEU H | 95 | 18.737 | 3.085 | 83.375 | 1.00 19.46 | H | Č |
| | A'TOM | 2409 | 0 | LEU H | 95 | 18.912 | 2.219 | 82.515 | 1.00 20.81 | H | |
| | MOTA | 2410 | СВ | LEU H | 95 | 17.117 | | | | | 0 |
| | | | | | | | 1.676 | 84.700 | 1.00 16.97 | H | C |
| | ATOM | 2411 | CG | LEU H | 95 | 18.301 | 1.013 | 85.430 | 1.00 19.81 | H | C |
| | | | | | | | | | | | |

| | ATOM | 2412 | CD1 LEU H | 951 | 18.891 | 2.007 | 86.390 | 1.00 26.56 | H | C |
|-----|------|------|-----------|------------|--------|--------|--------|------------|---|---|
| | MOTA | 2413 | CD2 LEU H | 95 | 17.837 | -0.192 | 86.136 | 1.00 17.57 | H | C |
| | MOTA | 2414 | N ASP H | 96 | 19.597 | 4.078 | 83.580 | 1.00 18.64 | H | N |
| | ATOM | 2415 | CA ASP H | 96 | 20.811 | 4.187 | 82.758 | 1.00 18.97 | H | С |
| 5 | MOTA | 2416 | C ASP H | 96 | 21.900 | 3.220 | 83.242 | 1.00 18.94 | H | С |
| • | ATOM | 2417 | O ASP H | 96 | 22.915 | 3.065 | 82.569 | 1.00 14.63 | H | 0 |
| | ATOM | 2418 | CB ASP H | 96 | 21.338 | 5.617 | 82.723 | 1.00 20.09 | Н | Č |
| | ATOM | 2419 | CG ASP H | 96 | 20.502 | 6.519 | 81.755 | 1.00 19.58 | H | č |
| | MOTA | 2420 | OD1 ASP H | 96 | 19.319 | 6.184 | 81.578 | 1.00 26.69 | H | Õ |
| 40 | | | | | 21.002 | 7.513 | 81.224 | 1.00 20.03 | H | ŏ |
| 10 | ATOM | 2421 | OD2 ASP H | 96 | 21.663 | 2.627 | 84.402 | 1.00 15.66 | H | И |
| | MOTA | 2422 | N GLY H | 97 | | | | | | |
| | ATOM | 2423 | CA GLY H | 97 | 22.574 | 1.601 | 84.922 | 1.00 16.17 | H | C |
| | MOTA | 2424 | C GLY H | 97 | 23.126 | 1.821 | 86.310 | 1.00 16.48 | H | C |
| | MOTA | 2425 | O GLY H | 97 | 23.064 | 2.935 | 86.841 | 1.00 14.75 | H | 0 |
| 15 | ATOM | 2426 | N TYR H | 98 | 23.737 | 0.782 | 86.887 | 1.00 12.61 | H | N |
| | MOTA | 2427 | CA TYR H | 98 | 24.259 | 0.958 | 88.226 | 1.00 13.48 | H | C |
| | MOTA | 2428 | C TYR H | 98 | 25.374 | 2.029 | 88.271 | 1.00 14.66 | H | C |
| | MOTA | 2429 | O TYR H | 98 | 25.598 | 2.639 | 89.299 | 1.00 15.42 | Н | 0 |
| | ATOM | 2430 | CB TYR H | 98 | 24.709 | -0.385 | 88.870 | 1.00 15.11 | H | C |
| 20 | MOTA | 2431 | CG TYR H | 98 | 25.762 | -1.194 | 88.104 | 1.00 12.19 | H | C |
| | MOTA | 2432 | CD1 TYR H | 98 | 27.123 | -1.116 | 88.450 | 1.00 18.17 | H | С |
| | ATOM | 2433 | CD2 TYR H | 98 | 25.384 | -2.089 | 87.124 | 1.00 12.48 | н | С |
| | ATOM | 2434 | CE1 TYR H | 98 | 28.089 | -1.955 | 87.822 | 1.00 18.60 | н | C |
| | ATOM | 2435 | CE2 TYR H | 98 | 26.330 | -2.917 | 86.489 | 1.00 8.78 | H | Č |
| 25 | MOTA | 2436 | CZ TYR H | 98 | 27.651 | -2.853 | 86.838 | 1.00 9.46 | H | č |
| 25 | | 2437 | OH TYR H | 98 | 28.553 | -3.723 | 86.277 | 1.00 13.71 | H | ŏ |
| | MOTA | | | 99 | 26.025 | 2.308 | 87.154 | 1.00 10.25 | H | Ŋ |
| | MOTA | 2438 | | | 27.038 | 3.382 | 87.160 | 1.00 10.23 | H | Ç |
| | ATOM | 2439 | CA TYR H | 99 | | | 86.874 | 1.00 11.42 | н | č |
| | ATOM | 2440 | C TYR H | 99 | 26.476 | 4.782 | | | | |
| 30 | ATOM | 2441 | O TYR H | 99 | 27.213 | 5.755 | 86.930 | 1.00 11.93 | H | 0 |
| | MOTA | 2442 | CB TYR H | 99 | 28.127 | 3.102 | 86.073 | 1.00 9.58 | H | C |
| | MOTA | 2443 | CG TYR H | 99 | 29.112 | 2.030 | 86.522 | 1.00 11.24 | H | Č |
| | ATOM | 2444 | CD1 TYR H | 99 | 29.940 | 2.265 | 87.613 | 1.00 16.63 | H | C |
| | MOTA | 2445 | CD2 TYR H | 99 | 29.206 | 0.785 | 85.850 | 1.00 15.72 | H | C |
| 35 | MOTA | 2446 | CE1 TYR H | 99 | 30.872 | 1.295 | 88.063 | 1.00 17.96 | H | C |
| | ATOM | 2447 | CE2 TYR H | 99 | 30.145 | -0.222 | 86.275 | 1.00 20.42 | H | C |
| | ATOM | 2448 | CZ TYR H | 99 | 30.951 | 0.069 | 87.386 | 1.00 16.74 | H | C |
| | MOTA | 2449 | OH TYR H | 99 | 31.813 | -0.917 | 87.795 | 1.00 14.93 | H | 0 |
| | MOTA | 2450 | N PHE H | 100 | 25.185 | 4.855 | 86.518 | 1.00 14.05 | H | N |
| 40 | ATOM | 2451 | CA PHE H | | 24.563 | 6.095 | 86.063 | 1.00 12.94 | H | C |
| | MOTA | 2452 | C PHE H | | 23.283 | 6.544 | 86.789 | 1.00 15.00 | H | C |
| | ATOM | 2453 | O PHE H | | 22.930 | 7.725 | 86.705 | 1.00 16.90 | н | 0 |
| | ATOM | 2454 | CB PHE H | | 24.268 | 5.977 | 84.529 | 1.00 13.53 | Н | C |
| | ATOM | 2455 | CG PHE H | | 25.550 | 5.835 | 83.677 | 1.00 12.84 | H | Č |
| 45 | MOTA | 2456 | CD1 PHE H | | 25.918 | 4.597 | 83.136 | 1.00 12.65 | н | Ċ |
| 40 | MOTA | 2457 | CD2 PHE H | | 26.353 | 6.921 | 83.426 | 1.00 15.24 | н | č |
| | ATOM | 2458 | CE1 PHE H | | 27.068 | 4.469 | 82.358 | 1.00 12.14 | Ĥ | č |
| | | | | | 27.515 | 6.797 | 82.639 | 1.00 14.00 | H | č |
| | MOTA | 2459 | CE2 PHE H | | 27.862 | 5.563 | 82.110 | 1.00 12.32 | H | č |
| FO | MOTA | 2460 | | | | 5.615 | 87.466 | 1.00 13.85 | H | N |
| 50 | MOTA | 2461 | N GLY H | | 22.604 | | | | | |
| | ATOM | 2462 | CA GLY H | | 21.381 | 5.986 | 88.197 | 1.00 12.56 | H | C |
| | MOTA | 2463 | C GLY H | | 20.108 | 6.047 | 87.364 | 1.00 13.56 | H | C |
| | MOTA | 2464 | O GLY H | | 20.105 | 5.714 | 86.192 | 1.00 16.72 | H | 0 |
| | MOTA | 2465 | N PHE H | | 19.013 | 6.516 | 87.980 | 1.00 14.22 | H | N |
| 55 | ATOM | 2466 | CA PHE H | | 17.722 | 6.639 | 87.266 | 1.00 16.09 | H | C |
| | MOTA | 2467 | C PHE H | 100B | 17.797 | 8.041 | 86.665 | 1.00 19.51 | H | C |
| | MOTA | 2468 | O PHE H | 100B | 17.537 | 9.028 | 87.347 | 1.00 18.58 | H | 0 |
| | MOTA | 2469 | CB PHE H | 100B | 16.579 | 6.550 | 88.321 | 1.00 15.67 | H | C |
| | MOTA | 2470 | CG PHE H | | 16.435 | 5.181 | 88.952 | 1.00 17.58 | H | С |
| 60 | MOTA | 2471 | CD1 PHE H | 100B | 16.614 | 5.011 | 90.323 | 1.00 12.85 | H | С |
| | ATOM | 2472 | CD2 PHE H | 100B | 16.074 | 4.069 | 88.177 | 1.00 13.17 | H | С |
| | ATOM | 2473 | CE1 PHE H | | 16.444 | 3.764 | 90.923 | 1.00 13.91 | Н | Ċ |
| | ATOM | 2474 | CE2 PHE H | | 15.903 | 2.799 | 88.792 | 1.00 12.44 | H | Č |
| | ATOM | 2475 | CZ PHE H | | 16.083 | 2.656 | 90.155 | 1.00 9.26 | H | č |
| 65 | ATOM | 2475 | N ALA H | | 18.098 | 8.123 | 85.364 | 1.00 20.24 | H | Ŋ |
| U.J | | | CA ALA H | | 18.375 | 9.418 | 84.778 | 1.00 20.24 | H | Ĉ |
| | ATOM | 2477 | | | 17.175 | 10.278 | 84.391 | 1.00 17.03 | H | Č |
| | MOTA | 2478 | C ALA H | | 17.295 | 11.489 | 84.348 | 1.00 17.03 | H | Ö |
| | MOTA | 2479 | O ALA H | 101 101 | | | | | H | č |
| | MOTA | 2480 | CB ALA H | TOT | 19.295 | 9.264 | 83.594 | 1.00 13.65 | п | C |

| | ATOM | 2481 | И | TYR H | 102 | 16.043 | 9.647 | 84.130 | 1.00 18.14 | Н | i N |
|------|--------------|--------------|------------|----------------|-----|------------------|------------------|------------------|--------------------------|----------|-----|
| | ATOM | 2482 | ĈA | TYR H | | 14.816 | 10.361 | 83.745 | 1.00 17.04 | Н | I C |
| | ATOM | 2483 | C | TYR H | 102 | 13.645 | 9.693 | 84.420 | 1.00 17.35 | H | |
| | ATOM | 2484 | 0 | TYR H | | 13.572 | 8.471 | 84.472 | 1.00 14.92 | H | |
| 5 | ATOM | 2485 | CB | TYR H | | 14.593 | 10.296 | 82.235 | 1.00 17.95 | H | |
| | ATOM | 2486 | CG | TYR H | | 15.585 | 11.140 | 81.523 81.028 | 1.00 20.25 1.00 20.01 | H H | |
| | MOTA | 2487 2488 | CD1 CD2 | | | 16.757 15.402 | 10.591 12.513 | 81.456 | 1.00 20.01 | H | |
| | ATOM ATOM | 2489 | CE1 | TYR H | | 17.747 | 11.421 | 80.471 | 1.00 16.24 | H | |
| 10 | MOTA | 2490 | CE2 | TYR H | | 16.372 | 13.343 | 80.911 | 1.00 15.52 | H | |
| | ATOM | 2491 | CZ | TYR H | | 17.537 | 12.782 | 80.419 | 1.00 17.92 | H | |
| | MOTA | 2492 | OH | TYR H | 102 | 18.475 | 13.602 | 79.832 | 1.00 32.99 | H | |
| | MOTA | 2493 | N | TRP H | | 12.728 | 10.512 | 84.921 | 1.00 17.03 | H | |
| | MOTA | 2494 | CA | TRP H | | 11.564 | 10.003 | 85.632 | 1.00 17.00 | H | |
| 15 | ATOM | 2495 | C | TRP H | | 10.299 | 10.565 | 85.009 84.472 | 1.00 15.31 1.00 18.72 | H H | |
| | ATOM ATOM | 2496 2497 | O CB | TRP H | | 10.306 11.595 | 11.676 10.459 | 87.110 | 1.00 18.72 | H | |
| | ATOM | 2498 | CG | TRP H | | 12.760 | 9.947 | 87.947 | 1.00 22.42 | H | |
| | ATOM | 2499 | | TRP H | | 14.090 | 10.198 | 87.721 | 1.00 10.35 | F | |
| 20 | MOTA | 2500 | CD2 | | | 12.685 | 9.164 | 89.135 | 1.00 13.24 | H | |
| | MOTA | 2501 | NE1 | | | 14.852 | 9.613 | 88.706 | 1.00 24.99 | F | |
| | MOTA | 2502 | CE2 | | | 14.024 | 8.968 | 89.590 | 1.00 11.38 | F | |
| | ATOM | 2503 | CE3 | | | 11.623 | 8.607 | 89.878 90.710 | 1.00 13.12 1.00 9.14 | <u> </u> | |
| O.E. | MOTA | 2504 2505 | CZ2 CZ3 | | | 14.328 11.925 | 8.251 7.888 | 91.015 | 1.00 13.82 | ŀ | |
| 25 | ATOM ATOM | 2506 | CH2 | | | 13.281 | 7.709 | 91.426 | 1.00 13.97 | Ī | |
| | MOTA | 2507 | N | GLY H | | 9.216 | 9.792 | 85.071 | 1.00 16.98 | F | |
| | MOTA | 2508 | CA | GLY H | 104 | 7.947 | 10.303 | 84.542 | 1.00 20.03 | ŀ | |
| | MOTA | 2509 | С | GLY H | | 7.258 | 11.169 | 85.604 | 1.00 22.00 | ŀ | |
| 30 | MOTA | 2510 | 0 | GLY H | | 7.886 | 11.535 | 86.606 | 1.00 22.60 | 0 F | |
| | ATOM | 2511 | N | ALA H | | 5.979 | 11.508 | 85.400 | 1.00 24.52 1.00 23.39 | I I | - |
| | MOTA | 2512 2513 | CA C | ALA H ALA H | | 5.284 4.649 | 12.344 11.524 | 86.356 87.468 | 1.00 23.39 | ŀ | |
| | ATOM ATOM | 2514 | Ö | ALA H | | 4.218 | 12.078 | 88.465 | 1.00 24.75 | F | |
| 35 | ATOM | 2515 | СВ | ALA H | | 4.185 | 13.220 | 85.606 | 1.00 24.94 | | H C |
| | ATOM | 2516 | N | GLY H | | 4.600 | 10.191 | 87.314 | 1.00 21.97 | F | H N |
| | ATOM | 2517 | CA | GLY H | | 4.128 | 9.196 | 88.266 | 1.00 23.66 | | I C |
| | MOTA | 2518 | С | GLY H | | 2.610 | 9.025 | 88.183 | 1.00 23.03 | | H C |
| 40 | MOTA | 2519 | 0 | GLY H | | 1.872 | 9.910 | 87.772 | 1.00 24.09 | H | |
| 40 | MOTA | 2520 2521 | N CA | THR H | | 2.160 0.727 | 7.813 7.542 | 88.554 88.566 | 1.00 22.71 1.00 21.91 | | H C |
| | MOTA MOTA | 2522 | CA | THR H | | 0.306 | 6.924 | 89.901 | 1.00 21.11 | | H C |
| | MOTA | 2523 | ŏ | THR H | | 0.862 | 5.939 | 90.367 | 1.00 18.20 | | O E |
| | ATOM | 2524 | ĊВ | THR H | | 0.421 | 6.574 | 87.423 | 1.00 27.94 | I | H C |
| 45 | MOTA | 2525 | OG1 | | | -0.995 | 6.432 | 87.297 | 1.00 33.93 | | 0 E |
| | MOTA | 2526 | CG2 | | | 1.030 | 5.202 | 87.728 | 1.00 17.61 | | H C |
| | ATOM | 2527 | N | LEU H | | -0.687 -1.066 | 7.564 7.139 | 90.541 91.886 | 1.00 24.58 1.00 25.53 | | H N |
| | MOTA MOTA | 2528 2529 | CA C | LEU H | | -1.862 | 5.831 | 91.887 | 1.00 21.65 | | H C |
| 50 | MOTA | 2530 | Ö | LEU H | | -2.801 | 5.630 | 91.129 | 1.00 23.64 | | O E |
| | ATOM | 2531 | ČВ | LEU H | | -1.900 | 8.252 | 92.519 | 1.00 30.90 | | H C |
| | MOTA | 2532 | CG | LEU H | 108 | -1.075 | 9.150 | 93.442 | 1.00 20.00 | | H C |
| | MOTA | 2533 | | LEU H | | -1.415 | 10.631 | 93.266 | 1.00 20.00 | | H C |
| | MOTA | 2534 | | LEU H | | -1.299 | 8.835 | 94.921 | 1.00 20.00 | | H C |
| 55 | MOTA | 2535 | N | VAL H VAL H | | -1.423 -2.177 | 4.903 3.669 | 92.760 92.946 | 1.00 22.28 1.00 22.76 | | H C |
| | MOTA ATOM | 2536 2537 | CA C | VAL H | | -2.662 | 3.531 | 94.390 | 1.00 25.97 | | H C |
| | ATOM | 2538 | Ö | VAL H | | -1.892 | 3.509 | 95.340 | 1.00 22.42 | | O H |
| | ATOM | 2539 | СB | VAL H | | -1.276 | 2.487 | 92.593 | 1.00 22.61 | | H C |
| 60 | MOTA | 2540 | | VAL H | | -1.965 | 1.180 | 92.982 | 1.00 12.42 | | H C |
| | MOTA | 2541 | CG2 | VAL H | 109 | -0.991 | 2.473 | 91.104 | 1.00 15.97 | | H C |
| | MOTA | 2542 | N | ALA H | | -3.995 | 3.473 | 94.541 | 1.00 27.50 | | H N |
| | MOTA | 2543 | CA | ALA H | | -4.549 | 3.344 | 95.883 | 1.00 34.16 | | H C |
| 65 | ATOM | 2544 2545 | C O | ALA H ALA H | | -5.218 -6.145 | $1.984 \\ 1.604$ | 96.096 95.393 | 1.00 30.55 1.00 28.32 | | H O |
| , | MOTA MOTA | 2545 | CB | ALA H | | -5.561 | 4.471 | 96.092 | 1.00 28.32 | | H C |
| | MOTA | 2547 | N | VAL H | | -4.788 | 1.231 | 97.090 | 1.00 29.84 | | H N |
| | ATOM | 2548 | CA | VAL H | 111 | -5.337 | ~0.096 | 97.338 | 1.00 31.80 | | H C |
| | ATOM | 2549 | C | VAL H | 111 | -6.192 | 0.068 | 98.562 | 1.00 31.94 | 3 | H C |

| | ATOM | 2550 | 0 | VAL H 11 | .1 | -5.686 | 0.211 | 99.660 | 1.00 31 | 65 | Н | 0 |
|----|--------------|--------------|-----------|----------------------|----|--------------------|------------------|-------------------|--------------------|--------------|--------|--------|
| | ATOM | 2551 | CB | VAL H 11 | 1 | -4.207 | -1.118 | 97.630 | 1.00 34 | | H | C |
| | MOTA | 2552 | | | | -4.820 | -2.488 | 97.985 | | .41 | H | C |
| - | ATOM | 2553 | | VAL H 11 | | -3.279 -7.506 | -1.246 | 96.368 98.345 | 1.00 27 1.00 33 | | H H | C N |
| 5 | MOTA MOTA | 2554 2555 | N CA | SER H 11 SER H 11 | | -7.506 -8.423 | $0.047 \\ 0.257$ | 98.343 | 1.00 33 | | н | C |
| | ATOM | 2556 | CA | SER H 11 | | -9.780 | -0.337 | 99.112 | 1.00 36 | | H | Č |
| | ATOM | 2557 | ŏ | SER H 11 | | -10.182 | -0.482 | 97.946 | 1.00 37 | | H | Ö |
| | MOTA | 2558 | CB | SER H 11 | L2 | -8.603 | 1.761 | 99.645 | 1.00 32 | | H | C |
| 10 | MOTA | 2559 | OG | SER H 11 | L2 | -9.559 | 2.071 | | | 5.84 | H | 0 |
| | MOTA | 2560 | N | ALA H 11 | L3 | -10.487 | -0.646 | 100.169 | 1.00 38 | 1.14 | H | N |
| | ATOM | 2561 2562 | CA | ALA H 11 ALA H 11 | | -11.824 -12.805 | -1.173 0.001 | 100.013 99.959 | 1.00 41 | | H H | C |
| | MOTA MOTA | 2563 | 0 | ALA H 11 | | -13.983 | -0.202 | 99.665 | | 2.01 | H | Ö |
| 15 | ATOM | 2564 | ČВ | ALA H 1 | | -12.160 | | 101.202 | 1.00 43 | | Н | Č |
| | MOTA | 2565 | N | ALA H 13 | | -12.325 | 1.216 | 100.256 | | 5.04 | H | N |
| | MOTA | 2566 | CA | ALA H 1 | | -13.182 | 2.403 | 100.240 | | 2.22 | H | C |
| | ATOM | 2567 | C | ALA H 11 | | -13.707 | 2.673 2.218 | 98.847 97.839 | 1.00 34 | 1.27 5.90 | H H | C |
| 20 | ATOM ATOM | 2568 2569 | O CB | ALA H 13 | | -13.135 -12.458 | 3.611 | | | 7.25 | н Н | C |
| 20 | MOTA | 2570 | И | ALA H 1 | | -14.798 | 3.431 | 98.796 | | 1.74 | H | N |
| | ATOM | 2571 | CA | ALA H 1 | | -15.460 | 3.725 | 97.537 | 1.00 3 | 7.80 | H | C |
| | MOTA | 2572 | С | ALA H 1 | | -15.153 | 5.077 | 96.946 | 1.00 3 | | H | C |
| | MOTA | 2573 | 0_ | ALA H 1 | | -15.027 | 6.068 | 97.652 | | 4.30 | H | 0 |
| 25 | MOTA | 2574 2575 | CB | ALA H 1: THR H 1: | | -16.987 -15.090 | 3.584 5.101 | 97.707 95.622 | 1.00 39 | | H H | N C |
| | ATOM ATOM | 2576 | N. CA | THR H 1 | 16 | -14.834 | 6.322 | 94.882 | 1.00 32 | | H | C |
| | ATOM | 2577 | C | THR H 1 | | -15.916 | 7.317 | 95.224 | 1.00 3 | | H | C |
| | ATOM | 2578 | 0 | THR H 1 | | -17.121 | 6.985 | 95.198 | 1.00 3 | | H | 0 |
| 30 | MOTA | 2579 | CB | THR H 1 | | -14.893 | 6.044 | 93.385 | 1.00 32 | | H | C |
| | ATOM | 2580 | OG1 | THR H 1: | | ~13.832 | 5.138 7.314 | 93.046 92.582 | 1.00 4: | | H H | 0 |
| | ATOM ATOM | 2581 2582 | CG2 N | THR H 1: | | -14.752 -15.514 | 8.528 | 95.594 | 1.00 3 | | H | И |
| | MOTA | 2583 | CA | THR H 1 | | ~16.507 | 9.569 | 95.901 | 1.00 34 | | H | Ĉ |
| 35 | ATOM | 2584 | C | THR H 1 | | -16.052 | 10.810 | 95.193 | 1.00 3 | 2.82 | H | C |
| | MOTA | 2585 | 0 | THR H 1 | | -14.886 | 11.181 | 95.309 | 1.00 3 | | H | 0 |
| | ATOM | 2586 | CB | THR H 1 | | -16.597 | 9.867 | 97.385 | 1.00 3 | | H | C |
| | MOTA | 2587 | OG1 | THR H 1: | | -16.771 -17.789 | 8.640 10.765 | 98.098 97.652 | 1.00 3 | 9.01 | H H | C O |
| 40 | MOTA ATOM | 2588 2589 | CG2 N | PRO H 1 | | -16.949 | 11.457 | 94.426 | | 3.70 | H | N |
| 40 | ATOM | 2590 | CA | PRO H 1 | | -16.564 | 12.668 | 93.702 | 1.00 3 | | H | Ĉ |
| | ATOM | 2591 | С | PRO H 1 | | -16.494 | 13.861 | 94.655 | 1.00 3 | | H | C |
| | MOTA | 2592 | 0 | PRO H 1 | | -17.221 | 13.927 | 95.623 | | 0.13 | H | 0 |
| 45 | ATOM | 2593 | CB | PRO H 1 | | ~17.684 ~18.908 | 12.821 12.369 | 92.664 93.472 | 1.00 3 | | H H | C |
| 45 | MOTA MOTA | 2594 2595 | CG CD | PRO H 1 | | -18.372 | 11.132 | 94.206 | 1.00 3 | | H | G |
| | ATOM | 2596 | N | PRO H 1 | | -15.633 | 14.837 | 94.362 | 1.00 3 | | H | N |
| | ATOM | 2597 | CA | PRO H 1 | 19 | -15.571 | 15.983 | 95.273 | 1.00 3 | | H | C |
| | MOTA | 2598 | C | PRO H 1 | 19 | -16.672 | 16.985 | 95.043 | 1.00 3 | | H | C |
| 50 | ATOM | 2599 | O | PRO H 1 | | -17.268 | 17.024 | 93.972 | 1.00 3 | | H H | C |
| | ATOM ATOM | 2600 2601 | CB CG | PRO H 1 PRO H 1 | | -14.241 -14.176 | 16.620 16.379 | 94.924 93.413 | 1.00 3 | | H | Č |
| | MOTA | 2602 | CD | PRO H 1 | | -14.588 | 14.917 | 93.327 | 1.00 3 | | H | č |
| | MOTA | 2603 | N | SER H 1 | | -16.914 | 17.818 | 96.050 | 1.00 3 | | H | N |
| 55 | ATOM | 2604 | CA | SER H 1 | | -17.822 | 18.941 | 95.888 | 1.00 2 | | H | C |
| | MOTA | 2605 | C | SER H 1 | | -16.869 | 20.135 | 95.805 | 1.00 2 | | H | C |
| | MOTA | 2606 2607 | 0 | SER H 1 SER H 1 | | -16.006 -18.763 | 20.275 19.081 | 96.642 97.078 | 1.00 2 | | H H | С О |
| | MOTA MOTA | 2608 | CB OG | SER H 1 | | -19.749 | 18.049 | 97.009 | 1.00 3 | | H | ŏ |
| 60 | ATOM | 2609 | N | VAL H 1 | | -17.007 | 20.969 | 94.776 | 1.00 2 | | H | N |
| | MOTA | 2610 | CA | VAL H 1 | 21 | -16.132 | 22.120 | 94.603 | 1.00 2 | 0.71 | H | С |
| | ATOM | 2611 | С | VAL H 1 | 21 | -16.877 | 23.374 | | 1.00 2 | | H | C |
| | MOTA | 2612 | 0 | VAL H 1 | | -17.939 | 23.654 | | 1.00 2 | | H | 0 |
| 65 | MOTA MOTA | 2613 2614 | CB CG1 | VAL H 1 VAL H 1 | | -15.651 -14.748 | 22.195 23.381 | 93.124 92.927 | 1.001 1.001 | | H H | C |
| 65 | ATOM | 2615 | | VAL H 1 | | -14.936 | 20.859 | 92.738 | 1.00 1 | | H | č |
| | ATOM | 2616 | N | TYR H 1 | | -16.349 | 24.129 | 95.962 | 1.00 2 | | H | N |
| | ATOM | 2617 | CA | TYR H 1 | 22 | -17.044 | 25.341 | 96.426 | 1.00 2 | 4.88 | H | C |
| | ATOM | 2618 | С | TYR H 1 | | -16.203 | 26.561 | 96.279 | 1.00 2 | 4.68 | H | С |

| | | | | | | | | | | | _ |
|----|--------------|--------------|----------------------|-----|--------------------|------------------|------------------|------------------|-------|--------|--------|
| | ATOM | 2619 | O TYR H | 122 | -15.032 | 26.548 | 96.577 | 1.00 2 | | H | O ~ |
| | MOTA | 2620 | CB TYR H | | -17.433 | 25.221 | 97.904 | 1.00 2 | | H | Ĉ |
| | ATOM | 2621 | CG TYR H | | -18.344 | 24.069 | 98.199 | | 9.23 | H | C |
| | ATOM | 2622 | CD1 TYR H | | -19.571 | 23.951 | 97.546 | | 5.06 | H | C |
| 5 | MOTA | 2623 | CD2 TYR H | | -18.003 | 23.103 | 99.135 | 1.00 2 | | H | C |
| | MOTA | 2624 | CE1 TYR H | | -20.425 | 22.898 | 97.825 | | 1.10 | H | C |
| | ATOM | 2625 | CE2 TYR H | | -18.861 | 22.040 | 99.426 | 1.00 2 | | H | C |
| | ATOM | 2626 | CZ TYR H | | -20.059 | 21.950 | 98.767 | 1.00 2 | | H | G |
| | ATOM | 2627 | OH TYR H | | -20.912 | 20.895 | 99.028 | 1.00 3 1.00 2 | | H | 0 |
| 10 | ATOM | 2628 | N PRO H | | -16.812 | 27.668 | 95.855 95.685 | 1.00 2 | | H H | C N |
| | MOTA | 2629 | CA PRO H | | -16.066 | 28.906 | 97.011 | 1.00 2 | | n H | C |
| | MOTA | 2630 | C PRO H O PRO H | | ~15.828 ~16.675 | 29.629 29.601 | 97.899 | 1.00 2 | | H | Ö |
| | MOTA | 2631 | O PRO H CB PRO H | | -16.971 | 29.723 | 94.767 | 1.00 2 | | H | ç |
| 45 | ATOM | 2632 | | | ~18.354 | 29.723 | 95.265 | 1.00 2 | | H | č |
| 15 | ATOM ATOM | 2633 2634 | CG PRO H CD PRO H | 123 | ~18.245 | 27.839 | 95.513 | 1.00 2 | | H | č |
| | ATOM | 2635 | N LEU H | | -14.671 | 30.279 | 97.127 | 1.00 2 | | H | Ŋ |
| | ATOM | 2636 | CA LEU H | | -14.326 | 31.043 | 98.325 | 1.00 2 | | Н | C |
| | ATOM | 2637 | C LEU H | | -14.143 | 32.505 | 97.922 | 1.00 2 | | H | Ċ |
| 20 | MOTA | 2638 | O LEU H | | -13.148 | 32.883 | 97.270 | 1.00 2 | 8.59 | H | 0 |
| | MOTA | 2639 | CB LEU H | | -13.026 | 30.503 | 98.959 | 1.00 2 | 4.13 | H | С |
| | ATOM | 2640 | CG LEU H | 124 | -13.138 | 29.021 | 99.352 | 1.00 2 | 5.03 | H | C |
| | MOTA | 2641 | CD1 LEU H | | -11.734 | 28.606 | 99.873 | 1.00 1 | | H | C |
| | MOTA | 2642 | CD2 LEU H | 124 | -14.254 | 28.781 | 100.416 | 1.00 1 | | H | C |
| 25 | ATOM | 2643 | N ALA H | | -15.139 | 33.328 | 98.272 | 1.00 3 | | H | Ñ |
| | ATOM | 2644 | CA ALA H | 125 | -15.087 | 34.755 | 97.956 | 1.00 3 | | H | Č |
| | ATOM | 2645 | C ALA H | | -15.210 | 35.537 | 99.281 | 1.00 3 | | H | C |
| | ATOM | 2646 | O ALA H | | ~15.840 | 35.057 | 100.198 | 1.00 3 1.00 3 | | H H | C O |
| 00 | ATOM | 2647 | CB ALA H | | -16.260 | 35.102 36.744 | 97.030 99.375 | 1.00 3 | | п Н | N |
| 30 | MOTA | 2648 | N PRO H CA PRO H | | -14.621 -14.664 | 37.596 | 100.585 | 1.00 4 | | H | Ç |
| | MOTA MOTA | 2649 2650 | CA PRO H C PRO H | | -16.007 | 38.205 | 100.986 | 1.00 5 | | H | č |
| | ATOM | 2651 | O PRO H | | -16.816 | 38.560 | 100.135 | | 3.07 | H | ŏ |
| | MOTA | 2652 | CB PRO H | | ~13.650 | 38.697 | 100.281 | 1.00 4 | | H | Č |
| 35 | ATOM | 2653 | CG PRO H | | -13.593 | 38.733 | 98.735 | 1.00 4 | | H | C |
| 00 | ATOM | 2654 | CD PRO H | | -13.652 | 37.277 | 98.392 | 1.00 4 | 7.77 | H | С |
| | ATOM | 2655 | N GLY H | | -16.210 | 38.352 | 102.299 | 1.00 5 | 8.90 | H | N |
| | MOTA | 2656 | CA GLY H | 127 | -17.427 | 38.964 | | 1.00 6 | | H | C |
| | MOTA | 2657 | C GLY H | 127 | -17.313 | 40.472 | 102.691 | 1.00 6 | 55.56 | H | C |
| 40 | MOTA | 2658 | O GLY H | | -16.226 | 40.950 | | 1.006 | | H | 0 |
| | MOTA | 2659 | OXT GLY H | | -18.294 | 41.197 | 102.962 | 1.00 6 | | H | 0 |
| | MOTA | 2660 | N ASN H | | -7.670 | 46.717 | 99.327 | 1.00 6 | | H | N |
| | MOTA | 2661 | CA ASN H | | -6.184 | 46.774 | 99.368 | 1.00 5 | | H | C |
| | ATOM | 2662 | C ASN H | | -5.627 | 46.469 46.230 | 98.005 97.068 | 1.00 5 | | H H | C |
| 45 | MOTA | 2663 | O ASN H CB ASN H | | -6.373 -5.588 | | 100.384 | 1.00 6 | | H | ç |
| | MOTA MOTA | 2664 2665 | CB ASN H | | -6.609 | | 101.017 | 1.00 6 | | H | č |
| | MOTA | 2666 | OD1 ASN H | | -6.246 | | 101.820 | 1.00 7 | | H | ŏ |
| | MOTA | 2667 | ND2 ASN H | | -7.882 | | 100.680 | 1.00 8 | | H | N |
| 50 | MOTA | 2668 | N SER H | | -4.312 | 46.486 | 97.891 | 1.00 4 | | H | N |
| | ATOM | 2669 | CA SER H | | -3.669 | 46.251 | 96.611 | 1.00 4 | | H | C |
| | MOTA | 2670 | C SER H | | -4.089 | 44.941 | 95.952 | 1.00 4 | | H | C |
| | MOTA | 2671 | O SER H | | -4.406 | 44.914 | 94.760 | 1.00 3 | | H | 0 |
| | MOTA | 2672 | CB SER H | | -2.146 | 46.294 | 96.819 | 1.00 4 | | H | C |
| 55 | ATOM | 2673 | OG SER H | | -1.411 | 45.905 | 95.669 | 1.00 5 | | H | 0 |
| | MOTA | 2674 | N MET H | | -4.095 | 43.852 | 96.725 | 1.00 4 | | H | N |
| | MOTA | 2675 | CA MET H | | -4.446 | 42.512 | 96.186 | 1.00 3 | | H | C |
| | ATOM | 2676 | C MET H | | -5.703 | 41.912 | 96.823 | 1.00 3 | | H H | C |
| 00 | ATOM | 2677 | O MET H | | -6.094 | 42.315 | 97.901 96.461 | 1.00 3 | | H | C |
| 60 | MOTA | 2678 2679 | CB MET H | | -3.300 -1.919 | 41.536 41.970 | 95.966 | 1.00 3 | | H | C |
| | ATOM | | SD MET H | | -1.916 | 42.012 | 94.167 | 1.00 4 | | H | s |
| | ATOM ATOM | 2680 2681 | CE MET H | | -1.602 | 40.237 | 93.761 | 1.00 4 | 15.32 | H | Č |
| | ATOM | 2682 | N VAL H | | -6.345 | 40.956 | 96.158 | 1.00 2 | 29.30 | H | Й |
| 65 | ATOM | 2683 | CA VAL H | | -7.479 | 40.275 | 96.789 | 1.00 2 | 29.61 | H | С |
| | ATOM | 2684 | C VAL H | 136 | -7.179 | 38.760 | 96.714 | 1.00 2 | | H | C |
| | MOTA | 2685 | O VAL H | 136 | -6.608 | 38.289 | 95.727 | 1.00 2 | | H | 0 |
| | MOTA | 2686 | CB VAL H | 136 | -8.853 | 40.549 | 96.112 | 1.00 2 | | H | C |
| | MOTA | 2687 | CG1 VAL H | 136 | -8.827 | 40.116 | 94.635 | 1.00 3 | 30.30 | H | С |

| | ATOM | 2688 | CG2 VAL H 13 | 5 | -9.967 | 39.759 | 96.854 | 1.00 19.18 | | H | С |
|------|------|------|---------------|----------|---------------------|--------|---------|------------|----|--------------|---|
| | ATOM | 2689 | N THR H 13' | | -7.508 | 38.028 | 97.776 | 1.00 26.58 | | | |
| | ATOM | 2690 | | | | | | | | H | N |
| | | | CA THR H 13 | | -7.299 | 36.573 | 97.756 | 1.00 27.60 | | H | С |
| | ATOM | 2691 | C THR H 13 | | -8.644 | 35.855 | 97.592 | 1.00 29.30 | | H | C |
| 5 | ATOM | 2692 | O THR H 13 | 7 | -9.628 | 36.183 | 98.269 | 1.00 28.40 | | H | 0 |
| | MOTA | 2693 | CB THR H 137 | 7 | -6.612 | 36.148 | 99.044 | 1.00 26.81 | | H | |
| | MOTA | 2694 | OG1 THR H 13 | | | | | | | | C |
| | | | | | -5.301 | 36.741 | 99.081 | 1.00 29.61 | | H | 0 |
| | MOTA | 2695 | CG2 THR H 13 | | -6.425 | 34.610 | 99.115 | 1.00 27.58 | | H | C |
| | ATOM | 2696 | N LEU H 138 | 3 | -8.696 | 34.910 | 96.665 | 1.00 28.45 | | H | N |
| 10 | ATOM | 2697 | CA LEU H 138 | | -9.875 | 34.117 | 96.390 | 1.00 23.40 | | | |
| | ATOM | 2698 | | | | | | | | H | C |
| | | | C LEU H 138 | | -9.475 | 32.658 | 96.580 | 1.00 23.57 | | H | C |
| | ATOM | 2699 | O LEU H 138 | 3 | -8.305 | 32.326 | 96.795 | 1.00 25.01 | | H | 0 |
| | MOTA | 2700 | CB LEU H 138 | 3 | -10.312 | 34.265 | 94.935 | 1.00 23.55 | | H | Č |
| | ATOM | 2701 | CG LEU H 138 | | -10.498 | | | | | | _ |
| 4 == | | | | | | 35.735 | 94.482 | 1.00 30.56 | | H | C |
| 15 | MOTA | 2702 | CD1 LEU H 138 | | -10.849 | 35.826 | 92.950 | 1.00 19.69 |] | H | С |
| | MOTA | 2703 | CD2 LEU H 138 | 3 | -11.628 | 36.350 | 95.312 | 1.00 35.20 | | H | C |
| | ATOM | 2704 | N GLY H 139 |) | -10.444 | 31.776 | 96.475 | 1.00 19.26 | | H | N |
| | ATOM | 2705 | CA GLY H 139 | | | | | | | | |
| | | | | | -10.060 | 30.370 | 96.580 | 1.00 21.12 | | H | C |
| | MOTA | 2706 | C GLY H 139 | | -11.156 | 29.404 | 96.169 | 1.00 22.32 | 1 | H | C |
| 20 | MOTA | 2707 | O GLY H 139 |) | -12.255 | 29.823 | 95.796 | 1.00 19.43 | 1 | H | 0 |
| | ATOM | 2708 | N CYS H 140 | | -10.847 | 28.117 | 96.262 | 1.00 19.11 | | H | N |
| | ATOM | 2709 | CA CYS H 140 | | | | | | | | |
| | | | | | -11.784 | 27.040 | 95.972 | 1.00 23.52 | | H | C |
| | MOTA | 2710 | C CYS H 140 | | -11.571 | 25.947 | 97.001 | 1.00 23.22 |] | H | C |
| | ATOM | 2711 | O CYS H 140 |) | -10.418 | 25.607 | 97.321 | 1.00 22.91 | 1 | H | 0 |
| 25 | ATOM | 2712 | CB CYS H 140 | } | -11.557 | 26.447 | 94.562 | 1.00 25.73 | | H | č |
| | ATOM | 2713 | SG CYS H 140 | | | | | | | | |
| | | | | | -12.544 | 27.321 | 93.297 | 1.00 44.80 | | H | S |
| | MOTA | 2714 | N LEU H 141 | | -12.676 | 25.397 | 97.521 | 1.00 21.53 |] | H | N |
| | MOTA | 2715 | CA LEU H 141 | _ | -12.622 | 24.289 | 98.512 | 1.00 20.48 | 1 | H | C |
| | ATOM | 2716 | C LEU H 141 | | -13.066 | 23.030 | 97.777 | 1.00 18.89 | | H | |
| 30 | ATOM | 2717 | | | | | | | | | C |
| 30 | | | O LEU H 141 | | -14.169 | 23.004 | 97.193 | 1.00 22.71 |] | H | 0 |
| | ATOM | 2718 | CB LEU H 141 | | -13.598 | 24.560 | 99.692 | 1.00 17.17 | 1 | H | С |
| | ATOM | 2719 | CG LEU H 141 | _ | -13.729 | 23.490 | 100.794 | 1.00 25.38 | | H | C |
| | MOTA | 2720 | CD1 LEU H 141 | | -12.371 | 23.264 | 101.553 | 1.00 25.22 | | | ä |
| | | | | | | | | | | H | C |
| ~~ | ATOM | 2721 | CD2 LEU H 141 | | -14.797 | 23.935 | 101.790 | 1.00 21.03 | 1 | H | C |
| 35 | ATOM | 2722 | N VAL H 142 | 2 | -12.205 | 22.007 | 97.771 | 1.00 15.03 | 1 | -1 | N |
| | ATOM | 2723 | CA VAL H 142 | 2 | -12.486 | 20.744 | 97.075 | 1.00 15.13 | | H | C |
| | ATOM | 2724 | C VAL H 142 | | -12.671 | 19.721 | 98.187 | | | | |
| | | 2725 | | | | | | 1.00 18.32 | | H | C |
| | ATOM | | O VAL H 142 | | -11.708 | 19.140 | 98.693 | 1.00 19.22 | I | H | 0 |
| | ATOM | 2726 | CB VAL H 142 | <u>.</u> | -11.293 | 20.370 | 96.194 | 1.00 16.12 | I | Ŧ | C |
| 40 | ATOM | 2727 | CG1 VAL H 142 | : | -11.611 | 19.084 | 95.365 | 1.00 16.05 | | H | C |
| | MOTA | 2728 | CG2 VAL H 142 | | -11.007 | 21.534 | 95.233 | 1.00 16.52 | | | |
| | | | | | | | | | | Ī | C |
| | ATOM | 2729 | N LYS H 143 | | -13.938 | 19.463 | 98.512 | 1.00 19.22 | | Ŧ | N |
| | ATOM | 2730 | CA LYS H 143 | , | -14.254 | 18.650 | 99.664 | 1.00 23.50 | F | -I | C |
| | ATOM | 2731 | C LYS H 143 | , | -14.891 | 17.303 | 99.486 | 1.00 23.95 | | I | Ċ |
| 45 | ATOM | 2732 | O LYS H 143 | | -15.787 | 17.124 | 98.656 | 1.00 28.68 | Ī | | ŏ |
| . • | ATOM | 2733 | | | | | | | | | |
| | | | | | -15.156 | | 100.574 | 1.00 21.98 | ŀ | Ŧ | C |
| | MOTA | 2734 | CG LYS H 143 | • | -15.507 | 18.917 | 101.941 | 1.00 25.06 | I | -I | С |
| | ATOM | 2735 | CD LYS H 143 | , | -16.282 | 19.991 | 102.758 | 1.00 28.37 | F | -T | C |
| | MOTA | 2736 | CE LYS H 143 | | -16.877 | | 104.058 | 1.00 28.90 | Ī | | č |
| 50 | ATOM | 2737 | NZ LYS H 143 | | -15.810 | | | | | | |
| 00 | | | | | | 10.790 | 104.927 | 1.00 44.68 | F | | N |
| | ATOM | 2738 | N GLY H 144 | | -14.419 | | 100.312 | 1.00 24.19 | F | Ŧ | N |
| | ATOM | 2739 | CA GLY H 144 | | -14.944 | 15.038 | 100.379 | 1.00 26.62 | F | 1 | С |
| | MOTA | 2740 | C GLY H 144 | | -14.856 | 14.128 | 99.180 | 1.00 27.65 | F | | Č |
| | MOTA | 2741 | O GLY H 144 | | | | | | | | |
| EE | | | | | -15.897 | 13.622 | 98.714 | 1.00 30.78 | F | | 0 |
| 55 | MOTA | 2742 | N TYR H 145 | | -13.635 | 13.914 | 98.690 | 1.00 26.76 | F | I | N |
| | ATOM | 2743 | CA TYR H 145 | , | -13.398 | 13.016 | 97.550 | 1.00 27.17 | F | Ŧ | C |
| | ATOM | 2744 | C TYR H 145 | | -12.535 | 11.814 | 97.920 | 1.00 29.53 | F | | č |
| | ATOM | 2745 | O TYR H 145 | | | | 00 070 | | | | |
| | | | | | -11.889 | 11.802 | 98.970 | 1.00 25.98 | ŀ | | 0 |
| | MOTA | 2746 | CB TYR H 145 | | -12.743 | 13.759 | 96.378 | 1.00 24.08 | ŀ | ł | С |
| 60 | MOTA | 2747 | CG TYR H 145 | | -11.357 | 14.306 | 96.683 | 1.00 28.06 | I | Ŧ | C |
| | MOTA | 2748 | CD1 TYR H 145 | | -10.204 | 13.586 | 96.338 | 1.00 30.37 | Î | | Č |
| | ATOM | 2749 | CD2 TYR H 145 | | -11.196 | | | | | | ~ |
| | | | | | | 15.553 | 97.283 | 1.00 22.50 | F | | С |
| | MOTA | 2750 | CE1 TYR H 145 | | _. -8.897 | 14.112 | 96.575 | 1.00 25.17 | F | I | C |
| | ATOM | 2751 | CE2 TYR H 145 | | -9.926 | 16.061 | 97.539 | 1.00 20.82 | I- | I | C |
| 65 | MOTA | 2752 | CZ TYR H 145 | | -8.793 | 15.356 | 97.184 | 1.00 28.20 | H | | Č |
| | MOTA | 2753 | | | | | | | | | |
| | | | | | -7.553 | 15.864 | 97.461 | 1.00 17.93 | H | | 0 |
| | MOTA | 2754 | N PHE H 146 | | -12.555 | 10.780 | 97.056 | 1.00 31.05 | H | I | N |
| | MOTA | 2755 | CA PHE H 146 | | -11.737 | 9.586 | 97.264 | 1.00 31.43 | H | Į. | C |
| | MOTA | 2756 | C PHE H 146 | | -11.753 | 8.812 | 95.960 | 1.00 32.08 | I. | | Č |
| | | | | | , | 0.014 | 55.500 | JZ.00 | r | | _ |

| | ATOM MOTA | 2757 2758 | O PHE H 146 CB PHE H 146 | -12.805 -12.306 | 8.697 8.690 | 95.328 98.359 | 1.00 36.16 1.00 29.02 | H H | |
|----|--------------|--------------|--------------------------------|--------------------|------------------|------------------|--------------------------|--------|-----|
| | MOTA | 2759 | CG PHE H 146 | -11.379 | 7.556 | 98.767 | 1.00 27.00 | H | |
| _ | ATOM | 2760 | CD1 PHE H 146 | -10.421 | 7.740 | 99.757 98.121 | 1.00 22.36 1.00 27.68 | H H | _ |
| 5 | MOTA | 2761 | CD2 PHE H 146 | -11.440 -9.550 | 6.334 6.755 | 100.091 | 1.00 27.00 | H | |
| | MOTA | 2762 2763 | CE1 PHE H 146 CE2 PHE H 146 | -10.541 | 5.323 | 98.464 | 1.00 27.29 | H | |
| | ATOM ATOM | 2763 | CZ PHE H 146 | -9.600 | 5.530 | 99.443 | 1.00 22.36 | H | |
| | MOTA | 2765 | N PRO H 147 | -10.591 | 8.321 | 95.527 | 1.00 27.57 | H | |
| 10 | ATOM | 2766 | CA PRO H 147 | -9.315 | 8.477 | 96.209 | 1.00 26.64 | H | |
| | ATOM | 2767 | C PRO H 147 | -8.572 | 9.704 | 95.669 | 1.00 26.21 | H | |
| | MOTA | 2768 | O PRO H 147 | -9.112 | 10.443 | 94.866 | 1.00 25.89 | H | |
| | MOTA | 2769 | CB PRO H 147 | -8.582 | 7.214 | 95.806 | 1.00 23.36 | H | |
| | ATOM | 2770 | CG PRO H 147 | -8.879 | $7.172 \\ 7.467$ | 94.377 94.332 | 1.00 25.94 1.00 26.74 | H H | |
| 15 | ATOM | 2771 2772 | CD PRO H 147 N GLU H 148 | -10.416 -7.335 | 9.901 | 96.128 | 1.00 26.28 | H | |
| | MOTA MOTA | 2773 | CA GLU H 148 | -6.490 | 10.963 | 95.562 | 1.00 29.14 | H | |
| | ATOM | 2774 | C GLU H 148 | -6.174 | 10.431 | 94.162 | 1.00 28.26 | Н | |
| | ATOM | 2775 | O GLU H 148 | -6.178 | 9.219 | 93.951 | 1.00 32.81 | H | |
| 20 | ATOM | 2776 | CB GLU H 148 | -5.206 | 11.084 | 96.344 | 1.00 27.60 | H | |
| | MOTA | 2777 | CG GLU H 148 | -5.450 | 11.628 | 97.701 | 1.00 28.15 | H | |
| | ATOM | 2778 | CD GLU H 148 | -4.209 | 12.176 | 98.294 98.735 | 1.00 46.58 1.00 56.93 | H H | |
| | MOTA | 2779 2780 | OE1 GLU H 148 OE2 GLU H 148 | -3.378 -4.080 | 11.332 13.441 | 98.294 | 1.00 30.93 | H | |
| 25 | MOTA MOTA | 2781 | N PRO H 149 | -5.806 | 11.313 | 93.216 | 1.00 28.64 | H | |
| 20 | ATOM | 2782 | CA PRO H 149 | -5.671 | 12.760 | 93.426 | 1.00 26.39 | H | C |
| | ATOM | 2783 | C PRO H 149 | -6.724 | 13.569 | 92.707 | 1.00 24.55 | H | |
| | MOTA | 2784 | O PRO H 149 | -7.597 | 13.026 | 92.035 | 1.00 23.88 | H | |
| | ATOM | 2785 | CB PRO H 149 | -4.314 | 13.034 | 92.809 | 1.00 28.35 | H H | |
| 30 | ATOM | 2786 | CG PRO H 149 | -4.455 | 12.232 10.913 | 91.462 91.932 | 1.00 20.74 1.00 28.56 | H | |
| | MOTA | 2787 2788 | CD PRO H 149 N VAL H 150 | -5.192 -6.627 | 14.890 | 92.868 | 1.00 23.29 | H | |
| | ATOM ATOM | 2789 | CA VAL H 150 | -7.448 | 15.809 | 92.113 | 1.00 19.21 | H | |
| | ATOM | 2790 | C VAL H 150 | -6.429 | 16.769 | 91.532 | 1.00 24.23 | H | |
| 35 | ATOM | 2791 | O VAL H 150 | -5.306 | 16.897 | 92.035 | 1.00 26.42 | H | |
| | ATOM | 2792 | CB VAL H 150 | -8.414 | 16.651 | 92.944 | 1.00 18.09 | H | |
| | MOTA | 2793 | CG1 VAL H 150 | -9.577 | 15.751 | 93.478 | 1.00 17.95 | H H | |
| | MOTA | 2794 | CG2 VAL H 150 | -7.665 | 17.369 17.441 | 94.096 90.471 | 1.00 10.71 1.00 24.63 | H | |
| 40 | MOTA | 2795 2796 | N THR H 151 CA THR H 151 | -6.811 -5.939 | 18.436 | 89.935 | 1.00 24.03 | H | |
| 40 | ATOM ATOM | 2797 | C THR H 151 | -6.700 | 19.742 | 90.049 | 1.00 28.78 | H | |
| | MOTA | 2798 | O THR H 151 | -7.915 | 19.765 | 89.869 | 1.00 26.29 | H | |
| | MOTA | 2799 | CB THR H 151 | | 18.153 | 88.481 | 1.00 31.70 | H | |
| | ATOM | 2800 | OG1 THR H 151 | | 18.052 | 87.694 | 1.00 43.95 | H | |
| 45 | MOTA | 2801 | CG2 THR H 151 | | 16.859 | 88.402 | 1.00 36.27 | H H | |
| | MOTA | 2802 | N VAL H 152 | | 20.808 22.127 | 90.364 90.436 | 1.00 26.62 1.00 25.23 | H | - |
| | ATOM ATOM | 2803 2804 | CA VAL H 152 C VAL H 152 | | 23.161 | 89.630 | 1.00 23.23 | H | |
| | MOTA | 2805 | O VAL H 152 | -4.544 | 23.228 | 89.792 | 1.00 27.04 | H | |
| 50 | MOTA | 2806 | CB VAL H 152 | -6.625 | 22.623 | 91.897 | 1.00 25.96 | H | |
| | MOTA | 2807 | CG1 VAL H 152 | -7.340 | 24.014 | 91.930 | 1.00 22.70 | H | |
| | MOTA | 2808 | CG2 VAL H 152 | | 21.609 | 92.784 | 1.00 25.04 | I. | |
| | MOTA | 2809 | N THR H 153 | | 23.915 | 88.736 88.048 | 1.00 20.60 1.00 23.67 | H | |
| EE | ATOM | 2810 | CA THR H 153 | | 24.996 26.211 | 88.132 | 1.00 23.07 | I. | |
| 55 | MOTA MOTA | 2811 2812 | C THR H 153 | | 26.061 | 88.565 | 1.00 25.71 | F | |
| | ATOM | 2813 | CB THR H 153 | | 24.659 | 86.551 | 1.00 24.28 | F | ı C |
| | ATOM | 2814 | OG1 THR H 153 | -6.632 | 24.412 | 85.889 | 1.00 25.91 | F | |
| | MOTA | 2815 | CG2 THR H 153 | | 23.435 | 86.450 | 1.00 19.31 | ŀ | |
| 60 | MOTA | 2816 | N TRP H 154 | | 27.393 | 87.752 | 1.00 28.43 | ŀ | |
| | MOTA | 2817 | CA TRP H 154 | | 28.600 | 87.754 86.342 | 1.00 32.03 1.00 30.20 | I I | |
| | MOTA | 2818 | C TRP H 154 | | 29.195 29.288 | 85.689 | 1.00 30.20 | ŀ | |
| | MOTA MOTA | 2819 2820 | O TRP H 154 | | | 88.748 | 1.00 23.01 | Ī | |
| 65 | ATOM | 2821 | CG TRP H 154 | | | 90.185 | 1.00 33.79 | ŀ | I C |
| | MOTA | 2822 | CD1 TRP H 154 | | 28.406 | 90.998 | 1.00 25.73 | I | ı C |
| | MOTA | 2823 | CD2 TRP H 154 | -7.800 | | | 1.00 32.12 | | i C |
| | MOTA | 2824 | NE1 TRP H 154 | | | | 1.00 21.18 1.00 27.40 | | A N |
| | MOTA | 2825 | CE2 TRP H 154 | | 28.900 | 92.239 | 1.00 47.40 | Г | |
| | | | | 1 7 1 | | | | | |

| | ATOM | 2826 | CE3 | TRP H | | -8.964 | 30.231 | 90.693 | 1.00 25.24 | | Н | C |
|----------------|--------------|--------------|------------|----------------|-------|------------------|------------------|------------------|--------------------------|---|--------|--------|
| | ATOM ATOM | 2827 2828 | CZ2 CZ3 | TRP H | | -8.608 -9.929 | 29.024 30.352 | 93.254 91.705 | 1.00 29.44 1.00 30.04 | | H H | C |
| | MOTA | 2829 | CH2 | TRP H | 154 | -9.737 | 29.748 | 92.972 | 1.00 24.77 | | H | Č |
| 5 | MOTA | 2830 | N | ASN H | | -8.144 | 29.560 | 85.867 | 1.00 30.30 | | H | N |
| | ATOM ATOM | 2831 2832 | CA C | ASN H ASN H | | -8.219 -7.488 | 30.047 29.181 | 84.479 83.443 | 1.00 37.67 1.00 37.85 | | H | C |
| | MOTA | 2833 | Ö | ASN H | | -6.758 | 29.686 | 82.593 | 1.00 37.83 | | H H | C |
| | MOTA | 2834 | СВ | ASN H | 155 | -7.740 | 31.496 | 84.413 | 1.00 34.75 | | H | Č |
| 10 | ATOM | 2835 | CG OD1 | ASN H | | -8.733 | 32.415 | 85.030 | 1.00 35.49 | | H | C |
| | ATOM ATOM | 2836 2837 | | ASN H ASN H | | -9.845 -8.376 | 31.980 33.683 | 85.382 85.170 | 1.00 44.08 1.00 45.82 | | H | O |
| | ATOM | 2838 | N | SER H | | -7.712 | 27.876 | 83.528 | 1.00 45.82 | | H H | N |
| | ATOM | 2839 | CA | SER H | 156 . | -7.123 | 26.916 | 82.612 | 1.00 36.58 | | H | C |
| 15 | MOTA | 2840 | C | SER H | | -5.612 | 26.997 | 82.592 | 1.00 36.12 | | H | C |
| | ATOM ATOM | 2841 2842 | O CB | SER H SER H | | -4.972 -7.672 | 26.657 27.141 | 81.592 81.200 | 1.00 38.51 1.00 37.40 | | H H | 0 |
| | ATOM | 2843 | OG | SER H | | -9.060 | 26.867 | 81.135 | 1.00 37.40 | | H | Ö |
| | MOTA | 2844 | N | GLY H | | -5.040 | 27.435 | 83.706 | 1.00 30.77 | | H | N |
| 20 | MOTA | 2845 | CA | GLY H | | -3.601 | 27.547 | 83.803 | 1.00 26.68 | | H | C |
| | ATOM ATOM | 2846 2847 | C O | GLY H | | -3.067 -1.869 | 28.929 29.140 | 83.534 83.698 | 1.00 29.62 1.00 27.32 | | H H | C |
| | MOTA | 2848 | N | SER H | | -3.940 | 29.878 | 83.157 | 1.00 27.52 | | n H | N |
| | MOTA | 2849 | CA | SER H | | -3.528 | 31.255 | 82.852 | 1.00 33.96 | | H | C |
| 25 | MOTA | 2850 | C | SER H | | -3.142 | 32.019 | 84.087 | 1.00 36.34 | | H | C |
| | ATOM ATOM | 2851 2852 | O CB | SER H | | -2.390 -4.652 | 32.981 32.041 | 84.026 82.153 | 1.00 41.32 1.00 32.92 | • | H H | O C |
| | MOTA | 2853 | OG | SER H | | -4.650 | 31.782 | 80.781 | 1.00 39.53 | | H | ŏ |
| | ATOM | 2854 | N | LEU H | | -3.668 | 31.584 | 85.217 | 1.00 39.25 | | H | N |
| 30 | MOTA | 2855 2856 | CA | LEU H | | -3.396 | 32.230 | 86.494 | 1.00 38.76 | | H | C |
| | ATOM ATOM | 2857 | C O | LEU H | | -2.548 -3.049 | 31.225 30.197 | 87.244 87.730 | 1.00 36.89 1.00 39.64 | | H H | C |
| | MOTA | 2858 | ČВ | LEU H | | -4.734 | 32.462 | 87.186 | 1.00 41.00 | | H | Č |
| | MOTA | 2859 | CG | LEU H | | -4.879 | 33.242 | 88.473 | 1.00 45.92 | | H | C |
| 35 | ATOM ATOM | 2860 2861 | | LEU H | | -3.662 -6.162 | 34.081 34.082 | 88.758 | 1.00 44.07 | | H | C |
| | ATOM | 2862 | N | SER H | | -0.162 -1.268 | 34.082 | 88.320 87.329 | 1.00 46.78 1.00 35.36 | | H H | C N |
| | MOTA | 2863 | CA | SER H | | -0.327 | 30.620 | 87.958 | 1.00 37.84 | | H | Ĉ |
| 40 | MOTA | 2864 | C | SER H | | 0.509 | 31.105 | 89.144 | 1.00 34.85 | | H | C |
| 40 | ATOM ATOM | 2865 2866 | O CB | SER H SER H | | 0.707 0.607 | 30.378 30.089 | 90.115 86.877 | 1.00 35.06 1.00 39.57 | | H | 0 |
| | MOTA | 2867 | OG | SER H | | 1.004 | 28.783 | 87.208 | 1.00 54.86 | | H H | C |
| | ATOM | 2868 | N | SER H | 161 | 1.037 | 32.308 | 89.080 | 1.00 33.71 | | H | N |
| 45 | MOTA | 2869 | CA | SER H | | 1.863 | 32.781 | 90.185 | 1.00 35.46 | | H | C |
| 45 | ATOM ATOM | 2870 2871 | C | SER H SER H | | 0.926 -0.237 | 33.209 33.538 | 91.324 91.084 | 1.00 33.85 1.00 35.17 | | H H | C O |
| | ATOM | 2872 | СВ | SER H | | 2.743 | 33.966 | 89.718 | 1.00 33.17 | | H | c |
| | MOTA | 2873 | OG | SER H | | 1.944 | 35.110 | 89.467 | 1.00 38.84 | | H | 0 |
| EO | MOTA | 2874 | N | GLY H | | 1.410 | 33.159 | 92.556 | 1.00 30.84 | | H | N |
| 50 | MOTA MOTA | 2875 2876 | CA C | GLY H | | 0.551 -0.598 | 33.550 32.579 | 93.666 93.971 | 1.00 33.82 1.00 34.76 | | H H | C |
| | MOTA | 2877 | ŏ | GLY H | | -1.590 | 32.931 | 94.634 | 1.00 38.65 | | H | ŏ |
| | MOTA | 2878 | N | VAL H | | -0.499 | 31.357 | 93.468 | 1.00 33.18 | | H | N |
| 55 | ATOM ATOM | 2879 2880 | CA C | VAL H | | -1.520 -0.920 | 30.356 | 93.748 | 1.00 27.52 | | H | C |
| 33 | ATOM | 2881 | 0 | VAL H | | 0.275 | 29.483 29.223 | 94.821 94.805 | 1.00 27.53 1.00 27.13 | | H H | C |
| | MOTA | 2882 | CB | VAL H | 163 | -1.803 | 29.435 | 92.508 | 1.00 28.90 | | H | Č |
| | ATOM | 2883 | | VAL H | | -2.545 | 28.168 | 92.958 | 1.00 26.60 | | H | C |
| 60 | ATOM ATOM | 2884 2885 | CG2 N | VAL H HIS H | | -2.650 -1.746 | 30.208 29.029 | 91.431 95.772 | 1.00 27.66 | | H | C |
| 0 0 | ATOM | 2886 | CA | HIS H | | -1.297 | 28.109 | 96.780 | 1.00 25.64 1.00 22.44 | | H H | G M |
| | MOTA | 2887 | C | HIS H | 164 | -2.280 | 26.960 | 96.853 | 1.00 20.69 | | H | Č |
| | ATOM | 2888 | 0 | HIS H | | -3.363 | 27.117 | 97.415 | 1.00 20.78 | | H | 0 |
| 65 | ATOM ATOM | 2889 2890 | CB CG | HIS H | | -1.242 -0.075 | 28.731 29.633 | 98.162 98.360 | 1.00 19.62 1.00 29.05 | | H H | C |
| | ATOM | 2891 | | HIS H | | 1.236 | 29.205 | 98.227 | 1.00 25.03 | | H | N C |
| | MOTA | 2892 | CD2 | HIS H | 164 | -0.020 | 30.951 | 98.653 | 1.00 31.28 | | H | Ĉ |
| | ATOM | 2893 | | HIS H | | 2.044 | 30.236 | 98.426 | 1.00 15.96 | | H | C |
| | MOTA | 2894 | NE2 | HIS H | T04 | 1.307 | 31.300 | 98.684 | 1.00 26.44 | | H | N |

| | | | | | | -1.932 | 25.808 | 96.287 | 1.00 | 19.73 | н | N |
|-----|--------------|--------------|---------|----------------|-----|--------------------|--------|--------------------|---------------------|-------|--------|--------|
| | ATOM | 2896 | CA | THR H | 165 | -2.866 | 24.680 | 96.434 | 1.00 | | H | Ĉ |
| | MOTA | 2897 | С | THR H | 165 | -2.371 | 23.869 | 97.622 | 1.00 | | H | Č |
| | ATOM | 2898 | 0 | THR H | 165 | -1.277 | 23.330 | 97.589 | 1.00 | 20.05 | H | 0 |
| 5 | MOTA | 2899 | CB | THR H | 165 | -2.913 | 23.856 | 95.113 | 1.00 | 18.44 | H | C |
| | ATOM | 2900 | OG1 | THR H | | -3.554 | 24.648 | 94.107 | 1.00 | | H | 0 |
| | MOTA | 2901 | CG2 | THR H | | -3.750 | 22.575 | 95.299 | 1.00 | 13.68 | H | C |
| | ATOM | 2902 | N | PHE H | | -3.181 | 23.752 | 98.677 | 1.00 | 15.64 | H | N |
| | ATOM | 2903 | CA | PHE H | | -2.747 | 23.042 | 99.857 | 1.00 | | H | C |
| 10 | MOTA | 2904 | C | PHE H | | -2.826 | 21.500 | 99.769 | 1.00 | | H | C |
| | ATOM | 2905 | 0 | PHE H | | -3.701 | 20.936 | 99.109 | 1.00 | | H | 0 |
| | ATOM | 2906 | СВ | PHE H | | -3.553 | | 101.085 | 1.00 | | H | C |
| | ATOM | 2907 | CG | PHE H | | -3.345 | 25.027 | | 1.00 | | H | C |
| | MOTA | 2908 | | PHE H | | -3.999 | | 100.633 | 1.00 | | H | C |
| 15 | ATOM | 2909 | | PHE H | | -2.386 | | 102.291 | 1.00 | 7.74 | H | C |
| | ATOM | 2910 | | PHE H | | -3.663 | | 100.804 | 1.00 | 7.46 | H | C |
| | MOTA | 2911 | | PHE H | | -2.056 | | 102.470 | 1.00 | | H | C |
| | ATOM | 2912 | CZ | PHE H | | -2.693 | | 101.721 | 1.00 | | H | C |
| 00 | ATOM | 2913 2914 | N | PRO H | | -1.914 | | 100.440 | 1.00 | | H | N |
| 20 | ATOM ATOM | 2915 | CA C | PRO H | | -1.971 -3.327 | | 100.401 100.950 | $\frac{1.00}{1.00}$ | | H H | C C |
| | ATOM | 2916 | Ö | PRO H | | -3.865 | | 100.930 | 1.00 | | п Н | Ö |
| | ATOM | 2917 | СВ | PRO H | | -0.854 | | 101.368 | 1.00 | | H | c |
| | ATOM | 2918 | CG | PRO H | | 0.133 | | 101.292 | 1.00 | | H | Č |
| 25 | ATOM | 2919 | CD | PRO H | | -0.790 | | 101.282 | 1.00 | | H | Č |
| 20 | ATOM | 2920 | N | ALA H | | -3.846 | | 100.377 | 1.00 | | H | N |
| | ATOM | 2921 | ĈA | ALA H | | -5.123 | | 100.818 | 1.00 | | H | Ĉ |
| | MOTA | 2922 | C | ALA H | | -4.982 | | 102.200 | 1.00 | | H | č |
| | ATOM | 2923 | Õ | ALA H | | -3.910 | | 102.574 | 1.00 | | H | ŏ |
| 30 | ATOM | 2924 | CB | ALA H | | -5.584 | 16.142 | 99.847 | 1.00 | | H | Č |
| | ATOM | 2925 | N | VAL H | | -6.066 | | 102.963 | 1.00 | | H | N |
| | MOTA | 2926 | CA | VAL H | | -6.062 | | 104.288 | 1.00 | | H | C |
| | ATOM | 2927 | С | VAL H | | -7.177 | | 104.330 | 1.00 | | H | Ċ |
| | ATOM | 2928 | 0 | VAL H | 169 | -8.269 | 15.272 | 103.881 | 1.00 | 27.25 | H | 0 |
| 35 | ATOM | 2929 | CB | VAL H | 169 | -6.329 | | 105.345 | 1.00 | 28.37 | H | C |
| | ATOM | 2930 | CG1 | VAL H | 169 | -6.454 | 16.372 | 106.715 | 1.00 | 29.42 | H | C |
| | ATOM | 2931 | CG2 | VAL H | 169 | -5.155 | 18.088 | 105.368 | 1.00 | 24.48 | H | C |
| | ATOM | 2932 | N | LEU H | 170 | -6.868 | | 104.896 | 1.00 | 32.34 | H | N |
| | MOTA | 2933 | CA | LEU H | | -7.797 | | 104.952 | 1.00 | 32.97 | H | C |
| 40 | ATOM | 2934 | C | LEU H | | -8.536 | | 106.248 | 1.00 | 35.04 | H | C |
| | MOTA | 2935 | 0 | LEU H | | -7.909 | | 107.305 | 1.00 | | H | 0 |
| | ATOM | 2936 | CB | LEU H | | -7.042 | | 104.807 | 1.00 | | H | С |
| | MOTA | 2937 | CG | rea H | | -7.913 | | 104.914 | 1.00 | | H | C |
| 4 - | ATOM | 2938 | | LEU H | | -8.703 | | 103.629 | 1.00 | | H | C |
| 45 | ATOM | 2939 | | LEU H | | -7.010 | | 105.199 | 1.00 | | H | C |
| | MOTA | 2940 | N | ALA H | | -9.866 | | 106.155 | 1.00 | | H | N |
| | ATOM | 2941 | CA | ALA H | | -10.744 | | 107.322 | 1.00 | | H | C |
| | ATOM | 2942 2943 | C | ALA H | | -11.937 | | 106.998 | 1.00 | | H | C |
| 50 | MOTA MOTA | 2943 | O CB | ALA H ALA H | | -12.513 -11.254 | | 105.922 107.735 | 1.00 | | H | 0 |
| 50 | ATOM | 2945 | N | SER H | | -12.268 | | 107.733 | 1.00 | | H H | C |
| | ATOM | 2946 | CA | SER H | | -13.386 | | 107.783 | 1.00 | | H | C |
| | MOTA | 2947 | C | SER H | | -13.438 | | 106.381 | 1.00 | | H | Č |
| | ATOM | 2948 | Õ | SER H | | -14.468 | | 105.680 | 1.00 | | H | õ |
| 55 | ATOM | 2949 | СВ | SER H | | -14.693 | | 108.097 | 1.00 | | H | č |
| 00 | ATOM | 2950 | OG | SER H | | -14.605 | | 109.313 | 1.00 | | H | ŏ |
| | ATOM | 2951 | N | ALA H | | -12.316 | | 105.955 | 1.00 | | H | Ň |
| | ATOM | 2952 | ĈA | ALA H | 173 | -12.221 | | 104.638 | 1.00 | | H | Ĉ |
| | ATOM | 2953 | C | ALA H | | -12.433 | | 103.459 | 1.00 | | H | Č |
| 60 | ATOM | 2954 | Ō | ALA H | | -12.644 | | 102.354 | 1.00 | | H | ŏ |
| | ATOM | 2955 | CB | ALA H | | -13.182 | | 104.518 | 1.00 | | H | Č |
| | ATOM | 2956 | N | LEU H | | -12.418 | | 103.674 | 1.00 | | H | Ň |
| | ATOM | 2957 | CA | LEU H | | -12.548 | | 102.523 | 1.00 | | H | C |
| | MOTA | 2958 | C | LEU H | 174 | -11.479 | | 102.637 | 1.00 | | H | Č |
| 65 | ATOM | 2959 | 0 | LEU H | | -11.151 | | 103.719 | 1.00 | | H | Ō |
| | MOTA | 2960 | CB | LEU H | 174 | -13.921 | | 102.465 | 1.00 | 32.78 | H | С |
| | ATOM | 2961 | CG | LEU H | | -15.150 | | 102.332 | 1.00 | | H | C |
| | MOTA | 2962 | | LEU H | | -16.442 | | 102.384 | 1.00 | | H | C |
| | ATOM | 2963 | CD2 | LEU H | 174 | -15.089 | 10.326 | 101.005 | 1.00 | 20.98 | H | C |

| | ATOM ATOM ATOM | 2964 2965 2966 | N TYR H 1 CA TYR H 1 C TYR H 1 | 75 -9. 75 -10. | 983 13.877 651 15.217 | 101.148 | 1.00 27.64 1.00 27.11 1.00 25.89 | Н Н Н | N C C |
|----|------------------------------|------------------------------|--|--|--|--|--|------------------|-------------|
| 5 | ATOM ATOM ATOM ATOM | 2967 2968 2969 2970 | O TYR H 1 CB TYR H 1 CG TYR H 1 CD1 TYR H 1 | .75 -9. .75 -8. | 092 13.601 129 12.491 | 100.499 100.185 100.404 101.119 | 1.00 22.59 1.00 28.71 1.00 33.19 1.00 36.50 | H H H H | 0 0 0 |
| 10 | ATOM ATOM ATOM | 2971 2972 2973 | CD2 TYR H 1 CE1 TYR H 1 CE2 TYR H 1 | .75 -8. .75 -6. .75 -7. | 411 11.209 065 11.654 540 10.161 | 99.935 101.376 100.172 | 1.00 30.21 1.00 36.87 1.00 42.67 | Н Н Н | CCC |
| | ATOM ATOM ATOM | 2974 2975 2976 | CZ TYR H 1 OH TYR H 1 N THR H 1 CA THR H 1 | .75 -5. .76 -10. | 552 9.325 025 16.282 | 100.895 101.168 101.641 101.373 | 1.00 46.88 1.00 52.45 1.00 24.24 1.00 24.99 | Н Н Н Н | 0 N C |
| 15 | ATOM ATOM ATOM ATOM | 2977 2978 2979 2980 | CA THR H 1 C THR H 1 O THR H 1 CB THR H 1 | .76 -9. .76 -8. | 248 18.510 234 18.373 | 101.109 101.772 | 1.00 22.35 1.00 22.32 1.00 23.22 | н н н | 000 |
| 20 | MOTA MOTA MOTA | 2981 2982 2983 | OG1 THR H 1 CG2 THR H 1 N LEU H 1 | .76 –12. .76 –11. .77 –9. | 527 17.519 531 19.677 312 19.378 | 0 102.692 7 102.381 8 100.112 | 1.00 31.74 1.00 10.30 1.00 22.69 | Н Н Н | И С О |
| | ATOM ATOM ATOM ATOM | 2984 2985 2986 2987 | CA LEU H 3 C LEU H 3 C LEU H 3 CB LEU H 3 | .77 -8. .77 -9. | 730 21.621 895 21.750 | 99.559 99.205 | 1.00 25.06 1.00 24.30 1.00 22.61 1.00 21.57 | H H H H | C C C C |
| 25 | ATOM ATOM ATOM | 2988 2989 2990 | CG LEU H 1 CD1 LEU H 1 CD2 LEU H 1 | 177 -7. 177 -7. | 270 19.745 486 21.147 957 19.177 | 97.374 96.826 96.740 | 1.00 26.70 1.00 30.91 1.00 15.94 | Н Н Н | С С |
| 30 | MOTA ATOM ATOM | 2991 2992 2993 | N SER H C CA SER H C C SER H C | L78 -8. L78 -7. | 866 22.631 247 23.977 121 24.563 | 7 99.247 3 98.404 | 1.00 22.75 1.00 17.84 1.00 21.14 | H H H | и С |
| | MOTA MOTA MOTA MOTA | 2994 2995 2996 2997 | O SER H COS SER SER SER SER SER SER SER SER SER SE | L78 -8. L78 -7. | 998 24.067 445 24.866 328 24.876 410 25.678 | 5 100.475 1 101.317 | 1.00 24.22 1.00 13.35 1.00 13.31 1.00 17.80 | Н Н Н Н | И С О |
| 35 | ATOM ATOM ATOM | 2998 2999 3000 | CA SER H C C SER H C | L79 -6. L79 -6. | 422 26.34° 798 27.83° 983 28.190 | 7 96.877 5 96.921 | 1.00 21.55 1.00 18.82 1.00 16.75 | Н Н Н | C C |
| 40 | ATOM ATOM ATOM | 3001 3002 3003 | CB SER H COG SER | 179 -5. 180 -5. | 515 25.829 567 26.519 800 28.67 | 94.582 7 97.141 | 1.00 15.41 1.00 21.64 1.00 17.88 | H H H | C O N |
| | ATOM ATOM ATOM ATOM | 3004 3005 3006 3007 | CA SER H C C SER H C O SER H C CB SER H C | 180 -5. 180 -4. | 028 30.113 301 30.722 302 30.163 458 30.694 | 96.003 95.518 | 1.00 21.70 1.00 24.16 1.00 26.15 1.00 14.18 | H H H H | 000 |
| 45 | ATOM ATOM ATOM ATOM | 3008 3009 3010 | OG SER H I N VAL H I CA VAL H I | 180 -4. 181 -5. | 048 30.663 809 31.862 165 32.572 | 1 98.488 2 95.544 | 1.00 22.63 1.00 24.76 1.00 28.32 | Н Н Н | 0 N C |
| 50 | ATOM ATOM ATOM | 3011 3012 3013 | C VAL H O VAL H CB VAL H | 181 -5. 181 -6. 181 -5. | 303 34.07 373 34.53 777 32.19 | 4 95.252 8 93.107 | 1.00 31.11 1.00 27.76 1.00 25.96 | H H H | 0 |
| | ATOM ATOM ATOM | 3014 3015 3016 | CG1 VAL H CG2 VAL H N THR H CA THR H | $ \begin{array}{rrr} 181 & -4. \\ 182 & -4. \\ \end{array} $ | 239 32.58 989 32.89 211 34.81 218 36.23 | 0 91.965 0 94.590 | 1.00 24.23 1.00 28.59 1.00 32.70 1.00 34.03 | Н Н Н Н | С С |
| 55 | ATOM ATOM ATOM ATOM | 3017 3018 3019 3020 | CA THR H C THR H O THR H CB THR H | 182 -4. 182 -3. | .005 37.02 .093 36.70 .128 36.55 | 0 93.627 7 92.850 | 1.00 36.50 1.00 37.98 1.00 31.37 | H H H | 000 |
| 60 | ATOM ATOM ATOM | 3021 3022 3023 | OG1 THR H CG2 THR H N VAL H | 182 -3 . 182 -3 . | .283 35.72 .195 38.02 .848 38.02 | 0 97.033 3 96.277 5 93.405 | 1.00 40.50 1.00 32.65 1.00 39.24 | Н Н Н | О С О |
| | MOTA ATOM ATOM | 3024 3025 3026 | CA VAL H C VAL H O VAL H | 183 -5 . 183 -5 . | .783 38.81 .049 40.27 .559 40.55 | 8 92.535 9 93.616 | 1.00 37.33 1.00 40.59 1.00 43.75 | Н Н Н | 0 0 0 |
| 65 | MOTA MOTA MOTA | 3027 3028 3029 | CB VAL H CG1 VAL H CG2 VAL H N PRO H | 183 -5 183 -7 | .858 38.32 .723 36.80 .238 38.61 .671 41.22 | 2 90.921 3 91.650 | 1.00 35.36 1.00 23.98 1.00 30.51 1.00 44.29 | н н н н | и С С |
| | ATOM ATOM ATOM | 3030 3031 3032 | N PRO H CA PRO H C PRO H | 184 -4 | .892 42.66 .376 42.98 | 3 91.903 | 1.00 43.69 1.00 45.05 | H H | C |

| | ATOM ATOM ATOM | 3033 3034 3035 | O CB CG | PRO H PRO H PRO H | 184 184 | -7.27 -4.38 -3.26 | 5 43 9 42 | .516 .323 .373 | 91.440 90.625 90.169 | $\frac{1.00}{1.00}$ | 45.22 43.90 42.32 | н н н | 0 0 |
|----|------------------------------|------------------------------|-----------------------|----------------------------------|-------------------|--------------------------------------|----------------------|------------------------------|--------------------------------------|------------------------------|----------------------------------|------------------|-------------|
| 5 | ATOM ATOM ATOM ATOM | 3036 3037 3038 3039 | CD CA C | PRO H SER H SER H SER H | 185 185 | -3.96 -6.63 -8.02 -8.81 | 9 43 9 44 | .020 .801 .159 .602 | 90.368 93.170 93.496 92.254 | 1.00 1.00 1.00 | 44.98 45.15 50.32 51.82 | H H H H | C N C |
| 10 | MOTA ATOM ATOM MOTA | 3040 3041 3042 3043 | O CB OG N | SER H SER H SER H SER H | 185 185 | -9.99 -8.06 -7.31 -8.14 | 6 45 0 45 | .277 .308 .024 .353 | 92.098 94.512 95.657 91.385 | 1.00 1.00 1.00 1.00 | 53.19 52.23 55.30 55.70 | H H H H | И О С |
| | ATOM ATOM ATOM | 3044 3045 3046 | CA C O | SER H SER H SER H | 186 186 186 | -8.74 -9.40 -10.57 | 4 45 8 44 0 44 | .896 .843 .989 | 90.158 89.270 88.896 | 1.00 1.00 1.00 | 58.70 61.29 61.19 | H H H | 0 C |
| 15 | ATOM ATOM ATOM ATOM | 3047 3048 3049 3050 | CB OG N CA | SER H SER H PRO H PRO H | 186 187 | -7.68 -6.73 -8.66 -9.08 | 2 47 0 43 | .646 .223 .793 | 89.357 90.221 88.889 88.056 | 1.00 | 59.11 58.60 62.65 61.57 | H H H H | О И С |
| 20 | ATOM ATOM ATOM | 3051 3052 3053 | C O CB | PRO H PRO H PRO H | 187 187 187 | -10.34 -11.04 -7.87 -6.77 | 9 41 2 41 2 41 | .921 .382 .765 | 88.486 87.645 88.089 87.954 | 1.00 1.00 1.00 | | H H H | 0 0 0 |
| 25 | ATOM ATOM ATOM ATOM | 3054 3055 3056 3057 | CG CD N CA | PRO H PRO H ARG H ARG H | 187 188 | -7.18 -10.65 -11.84 | 4 43 2 41 3 41 | .758 .826 .865 .137 | 88.953 89.779 90.192 | 1.00 | 65.51 58.01 53.46 | H H H H | С И С |
| | ATOM ATOM ATOM ATOM | 3058 3059 3060 3061 | C O CB CG | ARG H ARG H ARG H | 188 188 | -12.86 -12.51 -11.44 -11.88 | 2 42 0 39 | .986 .894 .920 | 90.932 91.687 91.041 90.466 | 1.00 | 53.17 55.75 51.65 47.14 | H H H H | 0000 |
| 30 | ATOM ATOM ATOM | 3062 3063 3064 | CD NE CZ | ARG H ARG H ARG H | 188 188 | -13.08 -13.20 -14.09 | 0 38 8 38 2 38 | .057 .806 .535 | 91.212 92.451 93.397 | 1.00 1.00 1.00 | 24.95 25.44 30.93 | H H H | C N C |
| 35 | MOTA MOTA MOTA | 3065 3066 3067 3068 | NH1 NH2 N CA | ARG H ARG H PRO H PRO H | 188 189 | -14.93 -14.13 -14.16 -14.69 | 7 39 4 41 | .526 .270 .714 .684 | 93.250 94.492 90.705 89.815 | $\frac{1.00}{1.00}$ | 29.87 29.13 49.03 50.12 | H H H H | N N C |
| | ATOM ATOM ATOM | 3069 3070 3071 | C O CB | PRO H PRO H PRO H | 189 189 | -14.84 -15.58 -16.04 | 4 41 2 40 5 40 | .144 .532 .378 | 88.361 87.599 90.432 | 1.00 1.00 1.00 | 54.80 54.44 49.09 | H H H | 0 C |
| 40 | ATOM ATOM ATOM | 3072 3073 3074 3075 | CG CD N | PRO H PRO H SER H SER H | 189 190 | -16.48 -15.24 -14.15 -14.25 | 6 42 8 42 | .712 .289 .220 .724 | 90.883 91.522 87.985 86.615 | 1.00 1.00 | 45.12 45.67 58.65 59.70 | H H H H | С С С |
| 45 | MOTA MOTA MOTA | 3076 3077 3078 | CA C O CB | SER H SER H SER H | 190 190 | -14.25 -13.72 -14.32 -13.47 | 1 41 9 41 | .670 .395 .041 | 85.646 84.604 86.453 | 1.00 | 60.48 | H H H | 000 |
| 50 | ATOM ATOM ATOM ATOM | 3079 3080 3081 3082 | OG N CA C | SER H GLU H GLU H | 191 191 | -12.07 -12.57 -11.95 -12.26 | 3 41 4 40 | .870 .101 .053 .765 | 86.607 85.992 85.196 85.952 | 1.00 | 60.08 57.13 55.55 53.43 | H H H H | О О О |
| 50 | ATOM ATOM ATOM ATOM | 3083 3084 3085 | O CB CG | GLU H GLU H | 191 191 | -12.20 -12.05 -10.44 -10.00 | 8 38 8 40 | .705 .691 .259 | 87.155 85.112 84.207 | 1.00 | 54.38 57.09 57.68 | H H H | С С |
| 55 | ATOM ATOM ATOM | 3086 3087 3088 | OE2 | GLU H GLU H GLU H THR H | 191 191 | -8.49 -7.77 -8.02 | 1 40 0 42 | .571 .548 .728 .753 | 84.234 84.309 84.179 85.243 | 1.00 1.00 | 73.34 73.73 81.17 50.94 | H H H H | O O N |
| 60 | ATOM ATOM ATOM ATOM | 3089 3090 3091 3092 | N CA C O | THR H THR H THR H | 192 192 | -12.74 -13.13 -12.01 -10.92 | 7 36 5 35 | .498 .608 | 85.243 85.877 86.408 85.861 | 1.00 1.00 | 48.18 44.64 42.83 | H H H | О С И |
| | MOTA ATOM MOTA | 3093 3094 3095 | CB OG1 CG2 | THR H THR H THR H | 192 192 192 | -13.98 -13.20 -15.16 | 3 35 8 35 2 36 | .681 .335 .508 | 84.920 83.770 84.481 | 1.00 1.00 1.00 | 47.39 52.75 48.68 | H H H | С С |
| 65 | ATOM ATOM ATOM ATOM | 3096 3097 3098 3099 | N CA C O | VAL H VAL H VAL H VAL H | 193 193 | -12.30 -11.34 -12.10 -13.12 | 6 33 8 32 | .884 .959 .663 | 87.494 88.096 88.285 88.932 | 1.00 | 38.76 35.65 30.66 30.71 | H H H H | О С И |
| | ATOM ATOM | 3100 3101 | CB | VAL H VAL H | 193 | -10.82 -9.89 | 1 34 | .477 | 89.469 90.119 | 1.00 | 36.30 40.07 | H H | C |

| | ATOM | 3102 | | VAL H | | -10.0 | | 35.750 | 89.253 | | | 36.63 | H | C |
|-----|--------------|--------------|------------|----------------|-----|----------------|-----|------------------|------------------|------|-----|----------------|--------|--------|
| | ATOM ATOM | 3103 3104 | N CA | THR H | | -11.6 -12.2 | | 31.584 30.298 | 87.698 87.766 | | | 27.25 31.84 | H H | N C |
| | ATOM | 3105 | C | THR H | | -11.3 | 13 | 29.199 | 88.150 | 1. | 00 | 30.56 | H | С |
| 5 | ATOM | 3106 | 0 | THR H | | -10.2 | | 29.164 | 87.619 86.365 | | | 35.10 | H H | 0 |
| | ATOM ATOM | 3107 3108 | CB OG1 | THR H | | -12.9 -13.8 | | 29.966 30.962 | 86.049 | | | 34.30 38.36 | н | Ö |
| | ATOM | 3109 | CG2 | THR H | | -13.5 | | 28.614 | 86.345 | | | 25.67 | H | C |
| | MOTA | 3110 | N | CYS H | | -11.6 | | 28.313 | 89.081 | | | 27.97 | H | И |
| 10 | ATOM ATOM | 3111 3112 | CA C | CYS H | | -10.7 -11.2 | | 27.222 25.979 | 89.424 88.670 | | | 28.84 28.13 | H H | C |
| | ATOM | 3113 | ŏ | CYS H | 195 | -12.4 | | 25.684 | 88.593 | 3 1. | 00 | 31.76 | H | 0 |
| | ATOM | 3114 | CB | CYS H | | -10.7 | | 26.924 | 90.934 | | | 27.33 | H | C |
| 15 | ATOM ATOM | 3115 3116 | SG N | CYS H ASN H | | -12.2 -10.3 | | 26.220 25.273 | 91.586 88.077 | | | 35.64 27.69 | H H | S N |
| 15 | ATOM | 3117 | CA | ASN H | | -10.6 | | 24.077 | 87.321 | | | 29.01 | H | C |
| | MOTA | 3118 | C | ASN H | 196 | -10.2 | | 22.871 | 88.114 | | | 26.91 | H | C |
| | ATOM ATOM | 3119 3120 | O CB | ASN H ASN H | | -9.0 -9.9 | | 22.668 24.089 | 88.365 85.974 | | | 23.66 31.51 | H H | C |
| 20 | ATOM | 3121 | CG | ASN H | | -9.8 | | 25.473 | 85.388 | | | 29.50 | H | č |
| | ATOM | 3122 | | ASN H | | -8.7 | | 26.090 | 85.385 | | | 25.64 | H | 0 |
| | ATOM ATOM | 3123 3124 | ND2 N | ASN H VAL H | | -10.9 -11.2 | | 25.972 22.047 | 84.887 88.475 | | | 34.55 24.98 | H H | N |
| | ATOM | 3125 | CA | VAL H | | -10.9 | | 20.869 | 89.290 | | | 23.37 | H | Ĉ |
| 25 | MOTA | 3126 | С | VAL H | | -11.3 | | 19.582 | 88.587 | | | 25.84 | H | C |
| | MOTA | 3127 3128 | O CB | VAL H VAL H | | -12.4 -11.8 | | 19.458 20.937 | 88.041 90.611 | | | 29.92 24.03 | H H | 0 |
| | ATOM ATOM | 3129 | | VAL H | | -11.5 | | 19.731 | 91.490 | | | 23.67 | H | Č |
| | MOTA | 3130 | | VAL H | | -11.4 | | 22.237 | 91.355 | | | 16.84 | H | C |
| 30 | MOTA | 3131 3132 | N CA | ALA H ALA H | | -10.4 | | 18.623 17.328 | 88.607 88.004 | | | 28.07 29.46 | H H | N C |
| | ATOM ATOM | 3133 | CA | ALA H | | -10.7 | | 16.237 | 88.999 | | | 29.74 | H | Č |
| | ATOM | 3134 | 0 | ALA H | 198 | -9.3 | 76 | 16.314 | 89.732 | | | 28.58 | H | 0 |
| 0.5 | MOTA | 3135 | CB | ALA H HIS H | | -9.9 -11.2 | | 17.125 15.224 | 86.666 89.035 | | | 31.83 32.53 | H H | C N |
| 35 | MOTA MOTA | 3136 3137 | N CA | HIS H | | -11.0 | | 14.078 | 89.902 | | | 33.86 | H | C |
| | ATOM | 3138 | C | HIS H | 199 | -11.2 | 232 | 12.847 | 89.032 | | | 37.42 | H | C |
| | MOTA | 3139 | 0 | HIS H | | -12.3 -12.0 | | 12.254 14.034 | 88.992 90.998 | | | 41.76 32.12 | H H | C O |
| 40 | MOTA MOTA | 3140 3141 | CB CG | HIS H | | -11.9 | | 12.867 | 91.895 | | | 31.49 | H | Č |
| | ATOM | 3142 | ND1 | HIS H | 199 | -12.9 | 52 | 12.004 | 92.184 | 11. | | 37.94 | H | N |
| | ATOM | 3143 | | HIS H | | -10.8 -12.5 | | 12.456 11.128 | 92.632 93.086 | | | 25.88 36.27 | H H | C |
| | ATOM ATOM | 3144 3145 | CE1 NE2 | HIS H | | -11.2 | | 11.384 | 93.379 | | | 27.41 | H | N |
| 45 | ATOM | 3146 | N | PRO H | | -10.1 | | 12.430 | 88.34 | | | 38.60 | H | N |
| | MOTA | 3147 3148 | CA | PRO H PRO H | | -10.2 -11.0 | | 11.270 10.047 | 87.453 87.933 | _ | | 39.66 41.49 | H H | C |
| | MOTA MOTA | 3148 | С 0 | PRO H | | -11.8 | | 9.493 | 87.180 | | | 43.64 | H | Ö |
| | ATOM | 3150 | CB | PRO H | 200 | -8.7 | 757 | 10.945 | 87.218 | В 1. | | 40.63 | H | C |
| 50 | MOTA | 3151 | CG CD | PRO H PRO H | | -8.0 -8.7 | | 12.314 12.876 | 87.320 88.552 | | | 40.85 40.30 | H H | C |
| | ATOM ATOM | 3152 3153 | N | ALA H | | -10.7 | | 9.620 | 89.16 | | | 41.88 | H | N |
| | MOTA | 3154 | CA | ALA H | 201 | -11.3 | | 8.424 | 89.70 | 4 1. | | 41.92 | H | C |
| | MOTA | 3155 3156 | С | ALA H ALA H | | -12.9 -13.4 | | 8.316 7.201 | 89.60° 89.62 | | | 44.22 47.89 | H H | C O |
| 55 | ATOM ATOM | 3157 | O CB | ALA H | | -10.9 | | 8.210 | 91.13 | | | 40.12 | H | č |
| | MOTA | 3158 | N | SER H | 202 | -13.6 | 502 | 9.448 | 89.483 | 3 1. | | 42.09 | H | И |
| | ATOM | 3159 | CA | SER H SER H | | -15.0 -15.4 | | 9.475 10.267 | 89.37 | | | 40.45 38.79 | H H | C |
| 60 | ATOM ATOM | 3160 3161 | C O | SER H | | -16.5 | | 10.725 | 87.93 | | | 39.19 | H | Ö |
| | MOTA | 3162 | CB | SER H | 202 | -15.6 | 582 | 10.171 | 90.59 | 9 1 | .00 | 42.08 | H | С |
| | ATOM | 3163 | OG | SER H | | -15.3 | | 11.576 | 90.61 87.24 | | | 36.22 36.91 | H H | N |
| | MOTA MOTA | 3164 3165 | N CA | SER H SER H | | -14.4 -14.0 | | 10.429 11.176 | 86.00 | | | 40.54 | H | C |
| 65 | MOTA | 3166 | C | SER H | 203 | -15.2 | 268 | 12.515 | 86.25 | 0 1 | .00 | 38.44 | H | C |
| | ATOM | 3167 | O | SER H | | -16.3 | | 12.919 | 85.49 85.00 | | | 40.82 | H H | 0 C |
| | ATOM ATOM | 3168 3169 | CB OG | SER H SER H | | -15.4 -14.9 | | 10.389 9.087 | 84.87 | | | 47.70 | H | Ö |
| | ATOM | 3170 | N | THR H | | -14. | | 13.222 | 87.28 | | | 35.03 | H | N |

| | MOTA MOTA MOTA MOTA | 3171 3172 3173 3174 | CA C O CB | THR H 204 THR H 204 THR H 204 THR H 204 | | -15.393 -14.544 -13.329 -15.537 | 14.530 15.686 15.696 14.741 | 87.585 87.034 87.168 89.112 | 1.00 34.07 1.00 33.24 1.00 35.71 1.00 33.83 | H | H H H | 0000 |
|----|--------------------------------------|--------------------------------------|----------------------------|---|------------------|---|--|--|--|-------------|-----------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM | 3175 3176 3177 3178 3179 | | THR H 204 THR H 204 ALA H 205 ALA H 205 ALA H 205 | | -16.255 -16.312 -15.204 -14.534 -15.453 | 13.646 15.999 16.653 17.840 18.995 | 89.687 89.393 86.407 85.880 86.202 | 1.00 35.82 1.00 34.28 1.00 34.41 1.00 38.94 1.00 40.07 | I 1 1 | H H H H H | 0 0 0 0 |
| 10 | ATOM ATOM ATOM ATOM ATOM | 3180 3181 3182 3183 3184 | O CB N CA | ALA H 205 ALA H 205 VAL H 206 VAL H 206 VAL H 206 | | -16.600 -14.322 -14.967 -15.767 -14.996 | 19.055 17.753 19.902 21.053 22.353 | 85.724 84.382 87.036 87.420 87.222 | 1.00 42.36 1.00 39.13 1.00 39.65 1.00 37.30 1.00 37.10 |]]] | H H H H H | 0 C N C |
| 15 | ATOM ATOM ATOM ATOM ATOM | 3185 3186 3187 3188 3189 | O CB CG1 | VAL H 206 VAL H 206 VAL H 206 VAL H 206 ASP H 207 | | -13.831 -16.186 -16.886 -17.098 -15.626 | 22.454 20.947 22.189 19.750 23.335 | 87.600 88.923 89.369 89.125 86.601 | 1.00 40.56 1.00 36.53 1.00 32.26 1.00 38.59 1.00 35.38 | 1 | H H H H H | и С С |
| 20 | ATOM ATOM ATOM ATOM ATOM | 3190 3191 3192 3193 3194 | CA C O CB CG | ASP H 207 ASP H 207 ASP H 207 ASP H 207 ASP H 207 | | -14.990 -15.871 -17.040 -14.957 -14.115 | 24.640 25.557 25.744 25.124 24.246 | 86.473 87.308 86.999 85.019 84.144 | 1.00 37.03 1.00 35.92 1.00 39.88 1.00 37.71 1.00 39.42 | | H H H H H | 00000 |
| 25 | ATOM ATOM ATOM ATOM ATOM | 3195 3196 3197 3198 3199 | OD1 | ASP H 207 ASP H 207 LYS H 208 LYS H 208 LYS H 208 | | -12.921 -14.656 -15.319 -16.095 -15.655 | 24.093 23.689 26.132 27.022 28.476 | 84.439 83.162 88.368 89.244 89.192 | 1.00 35.89 1.00 48.31 1.00 39.14 1.00 36.68 1.00 35.58 | | H H H H H | С О О |
| 30 | ATOM ATOM ATOM ATOM ATOM | 3200 3201 3202 3203 3204 | O CB CG CD CE | LYS H 208 LYS H 208 LYS H 208 LYS H 208 LYS H 208 | | -14.567 -16.005 -16.852 -17.728 -18.601 | 28.829 26.512 27.300 26.320 25.501 | 89.650 90.697 91.664 92.414 91.481 | 1.00 34.67 1.00 36.45 1.00 36.28 1.00 44.47 1.00 35.64 | • | H H H H H | 00000 |
| 35 | ATOM ATOM ATOM ATOM | 3205 3206 3207 3208 3209 | NZ N CA C | LYS H 208 LYS H 209 LYS H 209 LYS H 209 LYS H 209 | | -19.805 -16.488 -16.140 -16.346 -17.343 | 26.271 29.339 30.757 31.368 31.090 | 91.120 88.609 88.547 89.952 90.597 | 1.00 51.91 1.00 35.32 1.00 38.07 1.00 36.98 1.00 35.14 | | H H H H H | N C C O |
| 40 | MOTA MOTA MOTA MOTA MOTA MOTA | 3210 3211 3212 3213 3214 | CB CG CD CE NZ | LYS H 209 LYS H 209 LYS H 209 LYS H 209 LYS H 209 | ! ! | -17.057 -16.780 -18.026 -18.408 -19.364 | 31.497 32.990 33.806 33.666 34.788 | 87.562 87.526 87.127 85.683 85.268 | 1.00 38.43 1.00 38.76 1.00 42.22 1.00 47.62 1.00 49.98 | | H H H H H | C C C C |
| 45 | ATOM ATOM ATOM ATOM ATOM | 3215 3216 3217 3218 3219 | N CA C O CB | ILE H 210 ILE H 210 ILE H 210 ILE H 210 ILE H 210 |) } } | -15.398 -15.507 -16.341 -15.920 -14.079 | 32.176 32.814 34.106 34.951 33.178 | 90.408 91.720 91.545 90.751 92.307 | 1.00 34.13 1.00 34.36 1.00 36.70 1.00 36.92 1.00 30.96 | | Н Н Н Н Н | О С С |
| 50 | ATOM ATOM ATOM ATOM TER | 3220 3221 3222 3223 3224 | CG1 CG2 CD1 | ILE H 210 ILE H 210 ILE H 210 ILE H 210 ILE H 210 |)) }) | -13.188 -14.210 -13.895 -17.412 | 31.942 33.676 30.740 34.268 | 92.372 93.754 93.031 92.175 | 1.00 25.29 1.00 19.07 1.00 10.95 1.00 42.73 | | н н н н | 0000 |
| 55 | ATOM ATOM ATOM ATOM ATOM | 3225 3226 3227 3228 3229 | N CA C O CB | SER I SER I SER I SER I SER I | 7 7 7 | 14.834 16.214 16.170 15.109 17.091 | -3.003 -3.341 -3.928 -3.952 -2.097 | 64.812 65.271 66.678 67.298 65.247 | 1.00 41.42 1.00 43.47 1.00 40.84 1.00 48.28 1.00 40.12 | | I I I I | о С О |
| 60 | MOTA MOTA MOTA MOTA MOTA | 3230 3231 3232 3233 3234 | OG N CA C | SER I THR I STHR I STHR I | | 18.449 17.309 17.384 18.542 19.375 | -2.441 -4.405 -5.002 -4.314 -3.666 | 65.503 67.177 68.513 69.246 68.616 | 1.00 44.19 1.00 34.11 1.00 29.26 1.00 26.30 1.00 24.38 | | I I I I | 0 0 |
| 65 | ATOM ATOM ATOM ATOM ATOM | 3235 3236 3237 3238 3239 | CB OG: CG: N | THR I STATE I | 3 3 3 9 | 17.703 18.969 16.606 18.512 19.568 | -6.516 -6.713 -7.253 -4.390 -3.787 | 68.458 67.790 67.702 70.571 71.402 | 1.00 28.98 1.00 27.25 1.00 36.34 1.00 21.02 1.00 23.18 | | I I I I | С О С С |

| | ATOM | 3240 | C ALA I | 9 | 20.950 | -4.314 | 70.951 | 1.00 24.18 | I | С |
|----|--------------|--------------|------------------------|-----------------|--------------------|-------------------|------------------|--------------------------|--------|--------|
| | ATOM | 3241 | O ALA I | 9 | 21.937 | -3.569 | 70.892 | 1.00 20.92 | Ī | ŏ |
| | MOTA | 3242 | CB ALA I | 9 | 19.330 | -4.175 | 72.849 | 1.00 21.47 | I | C |
| | MOTA | 3243 | N FER I | 10 | 21.013 | -5.611 | 70.655 | 1.00 24.97 | I | N |
| 5 | ATOM | 3244 | CA LEU I | 10 | 22.307 | -6.193 | 70.237 | 1.00 26.56 | Ī | C |
| | ATOM | 3245 | C LEU I | 10 | 22.751 | -5.658 | 68.891 | 1.00 25.43 | I | C |
| | MOTA MOTA | 3246 3247 | O LEU I CB LEU I | 10 10 | 23.914 22.221 | -5.335 -7.732 | 68.675 70.202 | 1.00 19.53 1.00 28.67 | I | C O |
| | ATOM | 3248 | CG LEU I | 10 | 23.461 | -8.495 | 69.682 | 1.00 26.07 | I | C |
| 10 | MOTA | 3249 | CD1 LEU I | 10 | 24.700 | -8.085 | 70.501 | 1.00 20.03 | I | č |
| .0 | ATOM | 3250 | CD2 LEU I | 10 | 23.224 | -9.990 | 69.854 | 1.00 24.04 | Ī | Č |
| | MOTA | 3251 | N ARG I | 11 | 21.798 | -5.499 | 67.962 | 1.00 24.80 | Ī | N |
| | ATOM | 3252 | CA ARG I | 11 | 22.203 | -4.971 | 66.672 | 1.00 27.70 | I | С |
| | MOTA | 3253 | C ARG I | 11 | 22.757 | -3.549 | 66.827 | 1.00 26.39 | I | C |
| 15 | ATOM | 3254 | O ARG I | 11 | 23.758 | -3.173 | 66.224 | 1.00 21.33 | I | 0 |
| | ATOM | 3255 | CB ARG I | 11 | 20.991 | -4.942 | 65.706 | 1.00 29.11 | I | C |
| | MOTA | 3256 3257 | CG ARG I | 11 11 | 21.336 20.129 | -4.327 -4.428 | 64.341 63.388 | 1.00 37.83 1.00 59.35 | I | C |
| | MOTA MOTA | 3258 | CD ARG I NE ARG I | 11 | 19.798 | -4.426 -5.830 | 63.125 | 1.00 39.33 | I | И |
| 20 | MOTA | 3259 | CZ ARG I | 11 | 18.838 | -6.243 | 62.294 | 1.00 87.85 | Î | C |
| | ATOM | 3260 | NH1 ARG I | 11 | 18.628 | -7.546 | 62.116 | 1.00 88.83 | Ī | Ŋ |
| | ATOM | 3261 | NH2 ARG I | 11 | 18.078 | -5.355 | 61.640 | 1.00 93.94 | I | N |
| | ATOM | 3262 | N GLU I | 12 | 22.046 | -2.733 | 67.605 | 1.00 26.89 | I | N |
| | MOTA | 3263 | CA GLU I | 12 | 22.466 | -1.355 | 67.799 | 1.00 29.03 | I | C |
| 25 | MOTA | 3264 | C GLU I | 12 | 23.851 | -1.358 | 68.464 | 1.00 28.58 | Ĭ | C |
| | ATOM | 3265 | O GLU I | 12 | 24.695 | -0.578 | 68.088 | 1.00 30.04 | Ī | 0 |
| | ATOM ATOM | 3266 3267 | CB GLU I | 12 12 | $21.448 \\ 20.044$ | -0.564 -0.379 | 68.676 68.020 | 1.00 31.80 1.00 32.87 | I I | C |
| | ATOM | 3268 | CD GLU I | 12 | 20.170 | 0.154 | 66.634 | 1.00 32.07 | I | č |
| 30 | ATOM | 3269 | OE1 GLU I | 12 | 20.725 | 1.266 | 66.479 | 1.00 53.05 | Î | ŏ |
| | ATOM | 3270 | OE2 GLU I | 12 | 19.739 | -0.539 | 65.689 | 1.00 56.29 | Ī | ŏ |
| | MOTA | 3271 | N LEU I | 13 | 24.085 | -2.252 | 69.415 | 1.00 26.72 | I | N |
| | MOTA | 3272 | CA LEU I | 13 | 25.411 | -2.267 | 70.083 | 1.00 25.15 | Ţ | C |
| | MOTA | 3273 | C LEU I | 13 | 26.478 | -2.630 | 69.053 | 1.00 23.94 | I | C |
| 35 | MOTA | 3274 | O LEU I | 13 | 27.532 | -2.002 | 68.968 | 1.00 23.25 | Ī | 0 |
| | MOTA | 3275 | CB LEU I | 13 | 25.430 | -3.257 | 71.250 | 1.00 19.59 | Ĭ | C |
| | ATOM ATOM | 3276 3277 | CG LEU I CD1 LEU I | 13 13 | 26.822 27.527 | -3.465 -2.134 | 71.893 72.269 | 1.00 21.18 1.00 17.02 | I | C |
| | ATOM | 3277 | CD1 LEU I | 13 | 26.609 | -2.154 -4.357 | 73.128 | 1.00 17.02 | I | Č |
| 40 | ATOM | 3279 | N ILE I | 14 | 26.169 | -3.614 | 68.219 | 1.00 22.17 | Ī | N |
| | ATOM | 3280 | CA ILE I | $\overline{14}$ | 27.151 | -3.987 | 67.195 | 1.00 22.12 | Ī | C |
| | MOTA | 3281 | C ILE I | 14 | 27.462 | -2.824 | 66.272 | 1.00 24.29 | I | C |
| | MOTA | 3282 | O ILE I | 14 | 28.630 | -2.545 | 65.946 | 1.00 20.50 | I | 0 |
| | MOTA | 3283 | CB ILE I | 14 | 26.636 | -5.195 | 66.369 | 1.00 22.54 | I | C |
| 45 | ATOM | 3284 | CG1 ILE I | 14 | 26.703 | -6.427 | 67.261 | 1.00 21.93 | Ï | C |
| | ATOM ATOM | 3285 3286 | CG2 ILE I | 14 14 | 27.478 25.918 | -5.405 -7.632 | 65.142 66.756 | 1.00 25.41 1.00 8.06 | I I | C |
| | ATOM | 3287 | N GLU I | 15 | 26.418 | -2.123 | 65.839 | 1.00 21.20 | Ī | И |
| | ATOM | 3288 | CA GLU I | | 26.638 | -0.996 | 64.931 | 1.00 25.50 | I | Ĉ |
| 50 | ATOM | 3289 | C GLU I | 15 | 27.501 | 0.044 | 65.592 | 1.00 28.78 | I | C |
| | MOTA | 3290 | O GLU I | 15 | 28.384 | 0.635 | 64.951 | 1.00 27.98 | I | 0 |
| | MOTA | 3291 | CB GLU I | | 25.295 | -0.372 | 64.555 | 1.00 27.43 | I | C |
| | MOTA | 3292 | CG GLU I | 15 | 24.551 | -1.225 | 63.545 | 1.00 42.04 | Ξ | C |
| | ATOM | 3293 | CD GLU I | | 23.135 | -0.746 | 63.339 | 1.00 54.77 | I | C |
| 55 | ATOM | 3294 3295 | OE1 GLU I OE2 GLU I | | 22.369 22.795 | $-1.442 \\ 0.323$ | 62.633 63.896 | 1.00 58.59 1.00 59.54 | I | 0 |
| | ATOM ATOM | 3296 | N GLU I | | 27.273 | 0.323 | 66.892 | 1.00 25.33 | I | И |
| | ATOM | 3297 | CA GLU I | | 28.104 | 1.315 | 67.541 | 1.00 26.19 | Ĭ | C |
| | ATOM | 3298 | C GLU I | | 29.575 | 0.871 | 67.615 | 1.00 28.29 | I | Č |
| 60 | ATOM | 3299 | O GLU I | | 30.478 | 1.680 | 67.399 | 1.00 29.14 | I | 0 |
| | MOTA | 3300 | CB GLU I | 16 | 27.565 | 1.649 | 68.961 | 1.00 26.31 | I | C |
| | MOTA | 3301 | CG GLU I | | 28.461 | 2.581 | 69.830 | 1.00 20.48 | I | С |
| | ATOM | 3302 | CD GLU I | | 28.623 | 3.961 | 69.264 | 1.00 32.83 | Ī | C |
| C. | ATOM | 3303 | OE1 GLU I | | 27.908 | 4.295 | 68.291 | 1.00 40.64 | I | 0 |
| 65 | ATOM | 3304 | OE2 GLU I | | 29.472 | 4.734 -0.397 | 69.788 67.929 | 1.00 43.53 1.00 28.42 | I | O M |
| | ATOM ATOM | 3305 3306 | N LEU I CA LEU I | | 29.825 31.221 | -0.397 | 68.009 | 1.00 28.42 | I | N C |
| | ATOM | 3307 | C LEU I | | 31.904 | -0.791 | 66.626 | 1.00 28.23 | Ī | Č |
| | ATOM | 3308 | O LEU I | | 33.088 | -0.550 | 66.527 | 1.00 27.73 | Ī | ŏ |
| | | | | | | | | | | |

| | n | 2220 | CD 7 DII 7 | 1 17 | 21 071 | 2 277 | CO 501 | 1 00 26 55 | _ | C |
|----|--------------|--------------|------------------------|----------|------------------|-----------------------|------------------|--------------------------|--------|---|
| | ATOM | 3309 | CB LEU I | 17 | 31.271 | -2.277 | 68.521 69.921 | 1.00 26.55 | I | C |
| | ATOM | 3310 | CG LEU I | 17 17 | 30.675 30.866 | -2.476 -3.925 | 70.342 | 1.00 22.72 1.00 5.48 | I | C |
| | ATOM ATOM | 3311 3312 | CD1 LEU I CD2 LEU I | 17 | 31.304 | -3.925 -1.516 | 70.342 | 1.00 5.48 | ī | Č |
| 5 | ATOM | 3313 | N VAL I | 18 | 31.121 | -0.991 | 65.570 | 1.00 28.82 | Ī | Ŋ |
| 3 | ATOM | 3314 | CA VAL I | 18 | 31.638 | -0.900 | 64.202 | 1.00 26.07 | Ī | Ĉ |
| | ATOM | 3315 | C VAL I | 18 | 32.001 | 0.574 | 64.016 | 1.00 27.53 | Ī | Č |
| | ATOM | 3316 | O VAL I | 18 | 33.103 | 0.905 | 63.597 | 1.00 28.33 | I | Ó |
| | ATOM | 3317 | CB VAL I | 18 | 30.542 | -1.316 | 63.171 | 1.00 26.01 | I | C |
| 10 | ATOM | 3318 | CG1 VAL I | 18 | 30.970 | -0.908 | 61.741 | 1.00 23.17 | I | C |
| | ATOM | 3319 | CG2 VAL I | 18 | 30.355 | -2.841 | 63.203 | 1.00 25.17 | I | C |
| | ATOM | 3320 | N ASN I | 19 | 31.090 | 1.462 | 64.389 | 1.00 26.75 | I | N |
| | ATOM | 3321 | CA ASN I | 19 | 31.322 | 2.900 | 64.248 | 1.00 29.23 | I | С |
| | ATOM | 3322 | C ASN I | 19 | 32.602 | 3.414 | 64.906 | 1.00 32.04 | I | С |
| 15 | ATOM | 3323 | O ASN I | 19 | 33.333 | 4.206 | 64.313 | 1.00 35.66 | I | 0 |
| | MOTA | 3324 | CB ASN I | 19 | 30.153 | 3.700 | 64.826 | 1.00 25.97 | I | C |
| | ATOM | 3325 | CG ASN I | 19 | 28.965 | 3.675 | 63.923 | 1.00 30.76 | Ī | C |
| | ATOM | 3326 | OD1 ASN I | 19 | 29.064 | 3.142 | 62.834 | 1.00 41.11 | I | 0 |
| | MOTA | 3327 | ND2 ASN I | 19 | 27.830 | 4.230 | 64.362 | 1.00 36.69 | Ī | N |
| 20 | ATOM | 3328 | N ILE I | 20 | 32.881 | 2.953 | 66.120 | 1.00 33.02 | I I | N |
| | ATOM | 3329 | CA ILE I | 20 | 34.051 | 3.465 | 66.808 | 1.00 28.41 1.00 31.21 | I | C |
| | ATOM | 3330 | C ILE I | 20 | 35.341 | $2.745 \\ 3.188$ | 66.514 66.974 | 1.00 31.21 | Ī | Ö |
| | MOTA | 3331 3332 | O ILE I CB ILE I | 20 20 | 36.404 33.808 | 3.522 | 68.353 | 1.00 30.21 | I | C |
| 25 | ATOM | 3332 3333 | CB ILE I CG1 ILE I | 20 | 33.570 | $\frac{3.522}{2.114}$ | 68.912 | 1.00 27.04 | Ī | č |
| 20 | ATOM ATOM | 3334 | CG2 ILE I | 20 | 32.621 | 4.425 | 68.633 | 1.00 26.74 | Ī | č |
| | ATOM | 3335 | CD1 ILE I | 20 | 33.456 | 2.091 | 70.446 | 1.00 22.08 | Ī | č |
| | MOTA | 3336 | N THR I | 21 | 35.295 | 1.659 | 65.765 | 1.00 28.97 | Ī | N |
| | ATOM | 3337 | CA THR I | 21 | 36.542 | 0.961 | 65.468 | 1.00 37.12 | I | C |
| 30 | ATOM | 3338 | C THR I | 21 | 37.026 | 1.176 | 64.016 | 1.00 43.61 | I | С |
| 00 | ATOM | 3339 | O THR I | 21 | 38.030 | 0.547 | 63.631 | 1.00 41.22 | I | 0 |
| | ATOM | 3340 | CB THR I | 21 | 36.422 | -0.551 | 65.744 | 1.00 34.69 | I | С |
| | ATOM | 3341 | OG1 THR I | 21 | 35.269 | -1.073 | 65.083 | 1.00 32.38 | I | 0 |
| | ATOM | 3342 | CG2 THR I | 21 | 36.270 | -0.797 | 67.257 | 1.00 40.35 | I | C |
| 35 | ATOM | 3343 | OXT THR I | 21 | 36.409 | 1.993 | 63.291 | 1.00 55.16 | I | 0 |
| | MOTA | 3344 | N ALA I | 26 | 43.997 | 8.557 | 65.207 | 1.00 69.33 | I | N |
| | MOTA | 3345 | CA ALA I | 26 | 44.625 | 7.777 | 66.323 | 1.00 68.31 | I | C |
| | ATOM | 3346 | C ALA I | 26 | 43.714 | 6.622 | 66.754 | 1.00 64.43 | I | C |
| | ATOM | 3347 | O ALA I | 26 | 42.506 | 6.636 | 66.515 | 1.00 62.57 | Ī | 0 |
| 40 | MOTA | 3348 | CB ALA I | 26 | 44.911 | 8.711 | 67.544 | 1.00 68.87 | I | C |
| | ATOM | 3349 | N PRO I | 27 | 44.291 | 5.604 | 67.401 | 1.00 61.86 | I | N |
| | ATOM | 3350 | CA PRO I | 27 | 43.464 | 4.466 | 67.845 | 1.00 58.39 | Ţ | C |
| | ATOM | 3351 | C PRO I | 27 | 42.411 | 4.863 | 68.889 | 1.00 52.46 | I I | C |
| 45 | MOTA | 3352 3353 | O PRO I | 27 27 | 42.542 44.481 | 5.887 3.486 | 69.578 68.436 | 1.00 50.21 1.00 60.58 | Ī | C |
| 45 | ATOM | 3354 | CB PRO I CG PRO I | 27 | 45.851 | 3.951 | 67.829 | 1.00 64.15 | Ī | č |
| | MOTA MOTA | 3355 | CD PRO I | 27 | 45.700 | 5.452 | 67.814 | 1.00 61.04 | Ï | č |
| | ATOM | 3356 | N LEU I | 28 | 41.371 | 4.040 | 68.988 | 1.00 44.59 | Ī | N |
| | ATOM | 3357 | CA LEU I | 28 | 40.291 | 4.236 | 69.953 | 1.00 38.35 | I | Ĉ |
| 50 | ATOM | 3358 | C LEU I | 28 | 40.815 | 4.411 | 71.393 | 1.00 36.55 | I | C |
| • | MOTA | 3359 | O LEU I | 28 | 41.470 | 3.515 | 71.932 | 1.00 33.53 | I | 0 |
| | ATOM | 3360 | CB LEU I | 28 | 39.361 | 3.039 | 69.898 | 1.00 33.20 | I | С |
| | ATOM | 3361 | CG LEU I | 28 | 38.138 | 3.175 | 70.774 | 1.00 34.45 | I | C |
| | MOTA | 3362 | CD1 LEU I | 28 | 37.435 | 4.451 | 70.368 | 1.00 31.50 | I | C |
| 55 | MOTA | 3363 | CD2 LEU I | 28 | 37.243 | 1.936 | 70.659 | 1.00 37.17 | I | C |
| | MOTA | 3364 | N CYS I | 29 | 40.517 | 5.546 | 72.026 | 1.00 35.16 | I | N |
| | MOTA | 3365 | CA CYS I | 29 | 40.968 | 5.823 | 73.401 | 1.00 36.16 | I | C |
| | MOTA | 3366 | C CYS I | 29 | 42.480 | 5.581 | 73.512 | 1.00 38.10 | I | C |
| | MOTA | 3367 | O · CYS I | 29 | 43.005 | 5.144 | 74.564 | 1.00 39.22 | I | 0 |
| 60 | MOTA | 3368 | CB CYS I | 29 | 40.268 | 4.916 | 74.411 | 1.00 35.11 | I | С |
| | MOTA | 3369 | SG CYS I | 29 | 38.447 | 4.968 | 74.417 | 1.00 37.70 | I | S |
| | MOTA | 3370 | N ASN I | 30 | 43.169 | 5.894 | 72.425 | 1.00 40.14 | I | N |
| | MOTA | 3371 | CA ASN I | 30 | 44.602 | 5.679 | 72.333 | 1.00 39.35 | I | C |
| | MOTA | 3372 | C ASN I | 30 | 45.329 | 5.949 | 73.624 | 1.00 36.93 | I | C |
| 65 | MOTA | 3373 | O ASN I | 30 | 45.210 | 7.017 | 74.208 | 1.00 32.09 | I | 0 |
| | MOTA | 3374 | CB ASN I | 30 | 45.207 | 6.547 | 71.244 | 1.00 43.64 | I | C |
| | MOTA | 3375 | CG ASN I | 30 | 46.711 | 6.362 | 71.155 | 1.00 55.59 | Ī | C |
| | MOTA | 3376 | OD1 ASN I | 30 | 47.194 | 5.233 | 70.959 | 1.00 62.75 | I | 0 |
| | MOTA | 3377 | ND2 ASN I | 30 | 47.462 | 7.453 | 71.337 | 1.00 51.82 | I | N |
| | | | | | | | | | | |

| | ATOM | 3378 | N | GLY I | 31 | 46.074 | 4.952 | 74.075 | 1.00 38.03 | I | N |
|-----|--------------|--------------|------------|--------------------|----------|------------------|--------------------|------------------|--------------------------|--------|---------|
| | MOTA | 3379 | CA | GLY I | 31 | 46.821 | 5.085 | 75.306 | 1.00 39.13 | I | C |
| | ATOM | 3380 3381 | C O | GLY I GLY I | 31 31 | 46.164 46.842 | 4.380 4.002 | 76.488 77.439 | 1.00 39.21 1.00 43.77 | I I | C |
| 5 | MOTA ATOM | 3382 | И | SER I | 32 | 44.851 | 4.173 | 76.433 | 1.00 34.47 | I | N |
| Ū | ATOM | 3383 | CA | SER I | 32 | 44.168 | 3.551 | 77.558 | 1.00 32.83 | I | C |
| | MOTA | 3384 | C | SER I | 32 | 44.218 | 2.038 | 77.452 | 1.00 29.83 | I | C |
| | ATOM | 3385 | O | SER I SER I | 32 32 | 44.077 42.691 | $1.493 \\ 4.023$ | 76.377 77.612 | 1.00 31.08 1.00 31.53 | I I | C |
| 10 | MOTA MOTA | 3386 3387 | CB OG | SER I | 32 | 42.650 | 5.395 | 77.934 | 1.00 34.76 | Ï | ŏ |
| 10 | ATOM | 3388 | N | MET I | 33 | 44.379 | 1.376 | 78.587 | 1.00 27.38 | I | N |
| | ATOM | 3389 | CA | MET I | 33 | 44.446 | -0.073 | 78.662 | 1.00 24.36 | I | C |
| | ATOM | 3390 | C | MET I | 33 | 43.337 | -0.507 0.204 | 79.639 80.584 | 1.00 25.82 1.00 26.49 | I I | C |
| 15 | ATOM ATOM | 3391 3392 | O CB | MET I MET I | 33 33 | 43.031 45.777 | -0.501 | 79.265 | 1.00 26.43 | Ī | č |
| 13 | ATOM | 3393 | CG | MET I | 33 | 46.998 | 0.144 | 78.599 | 1.00 24.81 | I | С |
| | MOTA | 3394 | SD | MET I | 33 | 47.119 | -0.525 | 76.995 | 1.00 42.00 | I | S |
| | ATOM | 3395 | CE | MET I | 33 | 47.786 42.805 | -2.194 -1.705 | 77.366 79.425 | 1.00 17.53 1.00 21.73 | I I | C N |
| 20 | ATOM ATOM | 3396 3397 | N CA | VAL I VAL I | 34 34 | 42.805 | -2.252 | 80.243 | 1.00 21.73 | Ī | Ĉ |
| 20 | ATOM | 3398 | C | VAL I | 34 | 42.041 | -3.740 | 80.451 | 1.00 19.97 | I | С |
| | MOTA | 3399 | 0 | VAL I | 34 | 42.957 | -4.311 | 79.872 | 1.00 21.24 | Ī | 0 |
| | MOTA | 3400 | CB | VAL I | 34 | 40.355 | -2.169 -0.700 | 79.540 79.385 | 1.00 17.84 1.00 18.18 | I | C |
| 25 | ATOM ATOM | 3401 3402 | CG1 | VAL I | 34 34 | 39.972 40.407 | -2.897 | 78.187 | 1.00 13.18 | Ī | č |
| 25 | ATOM | 3403 | N N | TRP I | 35 | 41.232 | -4.380 | 81.264 | 1.00 20.73 | I | N |
| | ATOM | 3404 | CA | TRP I | 35 | 41.500 | -5.774 | 81.451 | 1.00 23.82 | I | C |
| | ATOM | 3405 | C | TRP I | 35 | 40.614 | -6.606 -6.168 | 80.556 80.060 | 1.00 22.12 1.00 25.30 | I I | С О |
| 30 | MOTA MOTA | 3406 3407 | O CB | TRP I TRP I | 35 35 | 39.561 41.341 | -6.148 | 82.905 | 1.00 25.50 | Ï | č |
| 30 | ATOM | 3408 | CG | TRP I | 35 | 40.032 | -5.862 | 83.480 | 1.00 27.26 | I | C |
| | ATOM | 3409 | CD1 | | 35 | 38.843 | -6.512 | 83.204 | 1.00 25.09 | I | C |
| | MOTA | 3410 | CD2 | | 35 | 39.775 | -4.979 | 84.581 84.106 | 1.00 28.63 1.00 29.68 | I | C N |
| 25 | MOTA MOTA | 3411 3412 | NE1 CE2 | | 35 35 | 37.854 38.402 | -6.089 -5.145 | 84.106 | 1.00 29.00 | Ī | C |
| 35 | ATOM | 3413 | CE3 | | 35 | 40.568 | -4.070 | 85.298 | 1.00 27.26 | Ī | C |
| | MOTA | 3414 | CZ2 | | 35 | 37.820 | -4.434 | 85.992 | 1.00 29.43 | I | C |
| | MOTA | 3415 | CZ3 | | 35 | 39.987 | -3.368 | 86.342 | 1.00 33.13 | I I | C |
| 40 | MOTA | 3416 3417 | CH2 | TRP I SER I | 35 36 | 38.623 41.057 | -3.553 -7.830 | 86.683 80.328 | 1.00 30.81 1.00 22.08 | I | N |
| 40 | ATOM ATOM | 3418 | N CA | SER I | 36 | 40.306 | -8.723 | 79.463 | 1.00 22.46 | I | C |
| | MOTA | 3419 | C | SER I | 36 | 39.083 | -9.330 | 80.132 | 1.00 22.65 | I | C |
| | ATOM | 3420 | 0 | SER I | 36 | 39.001 | -9.447 | 81.350 | 1.00 24.38 1.00 21.35 | I | C |
| 45 | ATOM ATOM | 3421 3422 | CB OG | SER I SER I | 36 36 | 41.211 41.750 | -9.882 -10.425 | 79.041 80.244 | 1.00 21.35 | Ī | Ö |
| 45 | ATOM | 3423 | N | ILE I | 37 | 38.119 | -9.702 | 79.315 | 1.00 22.95 | Ī | N |
| | ATOM | 3424 | CA | ILE I | 37 | | -10.426 | 79.841 | 1.00 25.36 | I | C |
| | ATOM | 3425 | C | ILE I | 37 | | -11.897 | 79.613 | 1.00 26.84 1.00 29.27 | I I | C |
| 50 | MOTA MOTA | 3426 3427 | O CB | ILE I ILE I | 37 37 | | -12.177 -10.086 | 78.737 79.094 | 1.00 25.27 | Ī | C |
| 50 | ATOM | 3428 | | 1 ILE I | 37 | 35.923 | -9.994 | 77.620 | 1.00 34.62 | Ī | С |
| | MOTA | 3429 | CG2 | S IPE I | 37 | 35.237 | -8.686 | 79.517 | 1.00 30.64 | I | C |
| | MOTA | 3430 | | 1 ILE I | 37 | 34.699 | -9.222 | 76.962 | 1.00 30.59 | I | C N |
| EE | ATOM | 3431 | N | ASN I ASN I | 38 38 | | -12.821 -14.232 | 80.361 80.225 | 1.00 30.34 1.00 34.97 | I | G 74 |
| 55 | ATOM ATOM | 3432 3433 | CA C | ASN I | 38 | | -15.281 | 79.957 | 1.00 35.10 | Ī | č |
| | MOTA | 3434 | ŏ | ASN I | 38 | 36.406 | -16.244 | 79.188 | 1.00 37.36 | I | 0 |
| | MOTA | 3435 | СВ | ASN I | 38 | | -14.611 | 81.512 | 1.00 39.38 | I | C |
| 00 | MOTA | 3436 | CG | | 38 38 | | -13.645 -13.509 | 81.796 80.975 | 1.00 50.58 1.00 56.26 | I | C O |
| 60 | MOTA MOTA | 3437 3438 | | 1 ASN I 2 ASN I | 38 | 39.173 | -13.305 | 82.949 | 1.00 56.07 | Ī | N |
| | ATOM | 3439 | N | LEU I | 39 | 35.064 | -15.116 | 80.589 | 1.00 32.58 | I | N |
| | MOTA | 3440 | CA | LEU I | 39 | 34.009 | -16.109 | 80.469 | 1.00 30.50 | I | C |
| 0.5 | ATOM | 3441 | C | LEU I | 39 | | -15.725 | 79.516 79.226 | 1.00 30.46 1.00 29.70 | I | C 0 |
| 65 | ATOM ATOM | 3442 3443 | O CB | LEU I | 39 39 | | -14.539 -16.349 | 81.840 | 1.00 29.70 | Ī | C |
| | ATOM | 3444 | CG | | 39 | | -16.668 | 82.986 | 1.00 35.60 | I | С |
| | MOTA | 3445 | CD: | 1 LEU I | 39 | 33.523 | -16.640 | 84.316 | 1.00 45.44 | I | C |
| | ATOM | 3446 | CD: | 2 LEU I | 39 | 34.963 | -18.037 | 82.724 | 1.00 39.91 | I | С |

| | ATOM | 3447 | N | THR I | 40 | 32.215 ~ | 16 720 | 79.028 | 1 00 20 11 | | |
|-----|------|------|------------------|-------|----|----------|---------|--------|------------|---|---|
| | ATOM | 3448 | CA | THR I | | 31.090 - | | | 1.00 32.11 | I | N |
| | ATOM | 3449 | C | THR I | | | | 78.137 | 1.00 36.92 | I | C |
| | ATOM | 3450 | Ö | | | 29.935 ~ | | 78.953 | 1.00 36.68 | I | С |
| 5 | MOTA | | | THR I | | 29.227 - | | 78.508 | 1.00 41.36 | I | 0 |
| 3 | | 3451 | CB | THR I | | 30.565 - | | 77.503 | 1.00 38.87 | I | С |
| | MOTA | 3452 | OG1 | | | 30.405 ~ | | 78.536 | 1.00 44.51 | I | 0 |
| | MOTA | 3453 | CG2 | | | 31.520 ~ | 18.325 | 76.432 | 1.00 38.41 | I | Č |
| | ATOM | 3454 | \mathbf{N} | ALA I | 41 | 29.757 ~ | -16.503 | 80.145 | 1.00 34.46 | I | N |
| | MOTA | 3455 | CA | ALA I | 41 | | 16.071 | 81.033 | 1.00 35.79 | Ī | C |
| 10 | MOTA | 3456 | C | ALA I | | | 14.655 | 81.599 | 1.00 33.79 | | |
| | ATOM | 3457 | ŏ | ALA I | | 30.012 - | 1/ 202 | | | I | C |
| | MOTA | 3458 | СВ | ALA I | | | | 82.031 | 1.00 31.37 | I | 0 |
| | MOTA | | | | | 28.522 ~ | 17.069 | 82.189 | 1.00 37.14 | I | C |
| | | 3459 | N | GLY I | | 27.831 - | | 81.582 | 1.00 28.18 | I | N |
| 4.5 | ATOM | 3460 | CA | GLY I | | 27.864 ~ | | 82.100 | 1.00 26.16 | I | С |
| 15 | ATOM | 3461 | С | GLY I | | 28.773 ~ | 11.607 | 81.290 | 1.00 25.89 | I | C |
| | MOTA | 3462 | 0 | GLY I | 42 | 29.338 ~ | 10.675 | 81.811 | 1.00 23.85 | Ī | ŏ |
| | MOTA | 3463 | N | MET I | 43 | | 11.910 | 80.003 | 1.00 27.06 | Ī | N |
| | ATOM | 3464 | CA | MET I | 43 | | 11.125 | 79.167 | 1.00 26.49 | | |
| | MOTA | 3465 | C | MET I | | | -9.613 | 79.089 | | I | C |
| 20 | ATOM | 3466 | ŏ | MET I | | | | | 1.00 25.63 | I | C |
| 20 | ATOM | 3467 | | | | | -8.806 | 79.072 | 1.00 24.70 | I | 0 |
| | | | CB | MET I | | 29.863 - | | 77.726 | 1.00 25.09 | 1 | C |
| | ATOM | 3468 | CG | MET I | | | 10.946 | 76.823 | 1.00 31.87 | I | C |
| | ATOM | 3469 | SD | MET I | | | 11.571 | 75.102 | 1.00 50.36 | I | S |
| | ATOM | 3470 | CE | MET I | 43 | 29.431 - | 10.913 | 74.580 | 1.00 49.83 | Ī | č |
| 25 | MOTA | 3471 | N | TYR I | 44 | | -9.239 | 78.967 | 1.00 23.56 | Ī | N |
| | ATOM | 3472 | CA | TYR I | 44 | | -7.799 | 78.843 | 1.00 21.86 | Ī | |
| | MOTA | 3473 | С | TYR I | 44 | | -7.096 | 80.124 | | | C |
| | ATOM | 3474 | ŏ | TYR I | 44 | | -6.028 | _ | 1.00 19.99 | I | C |
| | ATOM | 3475 | CB | TYR I | 44 | | | 80.088 | 1.00 23.39 | I | 0 |
| 30 | ATOM | | | | | | -7.549 | 78.655 | 1.00 23.84 | I | С |
| 30 | | 3476 | CG | TYR I | 44 | | -8.026 | 77.350 | 1.00 25.71 | I | C |
| | ATOM | 3477 | CD1 | - | | 26.263 | -7.427 | 76.154 | 1.00 25.80 | I | C |
| | ATOM | 3478 | CD2 | _ | 44 | 24.952 | -9.061 | 77.315 | 1.00 27.28 | I | C |
| | ATOM | 3479 | CE1 | TYR I | 44 | 25.733 | -7.842 | 74.947 | 1.00 27.01 | Ī | Č |
| | MOTA | 3480 | CE2 | TYR I | 44 | - | -9.498 | 76.100 | 1.00 22.75 | Ī | Ğ |
| 35 | ATOM | 3481 | CZ | TYR I | 44 | | -8.867 | 74.922 | 1.00 25.01 | | |
| | ATOM | 3482 | OH | TYR I | 44 | | -9.249 | | | I | C |
| | ATOM | 3483 | N | CYS I | 45 | | | 73.690 | 1.00 22.75 | I | 0 |
| | ATOM | | | | | | -7.724 | 81.245 | 1.00 17.09 | I | N |
| | | 3484 | CA | CYS I | 45 | | -7.120 | 82.510 | 1.00 17.82 | I | С |
| 40 | ATOM | 3485 | С | CYS I | 45 | | -7.059 | 82.631 | 1.00 16.25 | I | C |
| 40 | ATOM | 3486 | 0 | CYS I | 45 | 30.515 | -6.076 | 83.113 | 1.00 21.21 | I | ō |
| | ATOM | 3487 | $^{\mathtt{CB}}$ | CYS I | 45 | 27.928 | -7.903 | 83.689 | 1.00 15.24 | Ī | č |
| | ATOM | 3488 | SG | CYS I | 45 | | -7.936 | 83.883 | 1.00 20.73 | Ī | S |
| | ATOM | 3489 | N | ALA I | 46 | | -8.135 | 82.267 | 1.00 18.66 | | |
| | ATOM | 3490 | CA | ALA I | 46 | | -8.093 | 82.348 | | Ī | N |
| 45 | ATOM | 3491 | C | ALA I | 46 | | | | 1.00 17.71 | I | C |
| .0 | ATOM | 3492 | | | | | -7.009 | 81.432 | 1.00 19.91 | I | C |
| | | | 0 | ALA I | 46 | | -6.368 | 81.794 | 1.00 20.23 | I | 0 |
| | ATOM | 3493 | CB | ALA I | 46 | | -9.518 | 81.983 | 1.00 15.35 | I | C |
| | ATOM | 3494 | N | ALA I | 47 | 32.200 | -6.861 | 80.216 | 1.00 23.62 | I | N |
| | ATOM | 3495 | ca | ALA I | 47 | 32.684 | -5.845 | 79.286 | 1.00 22.12 | I | C |
| 50 | ATOM | 3496 | C | ALA I | 47 | | -4.476 | 79.896 | 1.00 21.78 | Ī | č |
| | ATOM | 3497 | 0 | ALA I | 47 | | -3.602 | 79.813 | 1.00 18.94 | | Č |
| | ATOM | 3498 | CB | ALA I | 47 | | -5.952 | | | I | 0 |
| | ATOM | 3499 | N | LEU I | 48 | | | 77.927 | 1.00 18.65 | I | C |
| | ATOM | 3500 | CA | | | | -4.290 | 80.481 | 1.00 21.70 | I | N |
| EE | | | | LEU I | 48 | 31.014 - | -2.995 | 81.145 | 1.00 21.03 | I | C |
| 55 | ATOM | 3501 | C | LEU I | 48 | | -2.745 | 82.292 | 1.00 21.18 | I | C |
| | MOTA | 3502 | 0 | LEU I | 48 | 32.589 - | -1.653 | 82.438 | 1.00 16.61 | I | 0 |
| | MOTA | 3503 | $^{\mathrm{CB}}$ | LEU I | 48 | 29.582 - | -3.040 | 81.727 | 1.00 21.70 | I | Č |
| | ATOM | 3504 | CG | LEU I | 48 | | -1.822 | 82.642 | 1.00 13.05 | Ī | C |
| | MOTA | 3505 | CD1 | LEU I | 48 | | -0.520 | 81.854 | 1.00 9.05 | Ī | |
| 60 | ATOM | 3506 | | LEU I | 48 | | -2.056 | 83.235 | | | C |
| | ATOM | 3507 | N | GLU I | 49 | | | | 1.00 15.13 | I | C |
| | ATOM | 3508 | CA | | | | -3.767 | 83.108 | 1.00 20.18 | I | N |
| | | | | GLU I | 49 | | -3.663 | 84.258 | 1.00 19.63 | I | C |
| | MOTA | 3509 | C | GLU I | 49 | | -3.275 | 83.786 | 1.00 20.55 | I | C |
| 05 | ATOM | 3510 | 0 | GLU I | 49 | | -2.512 | 84.439 | 1.00 26.90 | I | Ō |
| 65 | ATOM | 3511 | CB | GLU I | 49 | 33.226 - | -5.012 | 85.031 | 1.00 17.04 | I | Č |
| | MOTA | 3512 | CG | GLU I | 49 | 31.984 - | -5.184 | 85.968 | 1.00 20.14 | Ī | Č |
| | MOTA | 3513 | CD | GLU I | 49 | | -4.123 | 87.040 | 1.00 22.52 | Ī | G |
| | MOTA | 3514 | | GLU I | 49 | | -4.160 | 87.843 | 1.00 21.57 | I | |
| | ATOM | 3515 | | GLU I | 49 | | -3.244 | 87.073 | | | 0 |
| | | | ~ — <i></i> | | | J.L. 0/0 | J.44 | 07.073 | 1.00 10.29 | I | 0 |

| | ATOM | 3516 | N | SER I | 50 | 34.973 | -3.759 | 82.611 | 1.00 18.39 1.00 18.04 | I | | N C |
|-----|--------------|--------------|----------|----------------|----------|-------------------------|------------------|------------------|--------------------------|---|----------|--------|
| | MOTA | 3517 | CA | SER I | 50 | 36.307 | -3.428 -2.022 | 82.082 81.492 | 1.00 18.04 | I | | C |
| | MOTA | 3518 | C | SER I | 50 | 36.368 37.235 | -2.022 -1.228 | 81.848 | 1.00 18.38 | I | | õ |
| - | MOTA | 3519 | 0 | SER I SER I | 50 50 | 36.684 | -4.412 | 80.956 | 1.00 16.41 | Ĩ | | č |
| 5 | MOTA | 3520 3521 | CB OG | SER I SER I | 50 | 37.988 | -4.119 | 80.518 | 1.00 14.68 | Ī | | Ō |
| | MOTA MOTA | 3521 | N | LEU I | 51 | 35.399 | -1.714 | 80.618 | 1.00 19.34 | I | | N |
| | ATOM | 3523 | CA | LEU I | 51 | 35.374 | -0.436 | 79.913 | 1.00 17.71 | I | | C |
| | ATOM | 3524 | C | LEU I | 51 | 34.994 | 0.798 | 80.754 | 1.00 19.46 | I | : | C |
| 10 | ATOM | 3525 | Ö | LEU I | 51 | 35.371 | 1.923 | 80.412 | 1.00 21.21 |] | • | 0 |
| 10 | ATOM | 3526 | СВ | LEU I | 51 | 34.421 | -0.552 | 78.686 | 1.00 16.17 |] | | С |
| | ATOM | 3527 | CG | LEU I | 51 | 35.014 | -1.455 | 77.585 | 1.00 11.29 |] | | C |
| | ATOM | 3528 | | LEU I | 51 | 34.002 | -1.641 | 76.483 | 1.00 7.04 | 3 | | С |
| | ATOM | 3529 | CD2 | | 51 | 36.271 | -0.787 | 76.972 | 1.00 14.57 |] | | С |
| 15 | ATOM | 3530 | N | ILE I | 52 | 34.326 | 0.582 | 81.875 | 1.00 18.04 |] | | N |
| | ATOM | 3531 | CA | ILE I | 52 | 33.927 | 1.732 | 82.725 | 1.00 16.93 | | | C |
| • | MOTA | 3532 | С | ILE I | 52 | 35.161 | 2.394 | 83.304 | 1.00 17.40 | | [| C |
| | MOTA | 3533 | 0 | ILE I | 52 | 35.133 | 3.574 | 83.726 | 1.00 22.32 | | [| 0 |
| | ATOM | 3534 | CB | ILE I | 52 | 32.981 | 1.272 | 83.897 | 1.00 17.81 | | [| C |
| 20 | MOTA | 3535 | CG1 | | 52 | 32.253 | 2.493 | 84.538 | 1.00 21.78 1.00 9.73 | | [[| C |
| | ATOM | 3536 | CG2 | | 52 | 33.789 | 0.520 | 84.971 | 1.00 9.73 1.00 8.98 | | [| C |
| | ATOM | 3537 | | ILE I | 52 | 31.212 | 3.105 1.649 | 83.597 83.374 | 1.00 22.00 | | [| N |
| | ATOM | 3538 | Ŋ | ASN I | 53 | 36.272 37.493 | 2.243 | 83.923 | 1.00 22.00 | | [| Ĉ |
| 0.5 | ATOM | 3539 | CA | ASN I ASN I | 53 53 | 38.211 | 3.184 | 82.999 | 1.00 21.40 | | [| Ċ |
| 25 | ATOM | 3540 | C | ASN I | 53 | 39.138 | 3.887 | 83.431 | 1.00 23.95 | | <u> </u> | ō |
| | ATOM | 3541 3542 | O CB | ASN I | 53 | 38.459 | 1.157 | 84.358 | 1.00 18.16 | | Γ | C |
| | ATOM ATOM | 3543 | CG | ASN I | 53 | 37.914 | 0.385 | 85.511 | 1.00 29.89 | | Γ | C |
| | ATOM | 3544 | | ASN I | 53 | 37.311 | 0.977 | 86.434 | 1.00 31.88 | | Γ | 0 |
| 30 | MOTA | 3545 | | ASN I | 53 | 38.068 | -0.941 | 85.467 | 1.00 41.94 | | Ε | N |
| 00 | ATOM | 3546 | N | VAL I | 54 | 37.781 | 3.241 | 81.733 | 1.00 23.83 | : | ŗ | N |
| | ATOM | 3547 | CA | VAL I | 54 | 38.471 | 4.131 | 80.784 | 1.00 25.45 | | Γ | C |
| | ATOM | 3548 | C | VAL I | 54 | 38.204 | 5.591 | 81.101 | 1.00 29.82 | | Ι | C |
| | ATOM | 3549 | 0 | VAL I | 54 | 37.062 | 5.987 | 81.206 | 1.00 31.49 | | I | 0 |
| 35 | MOTA | 3550 | CB | VAL I | 54 | 38.064 | 3.832 | 79.306 | 1.00 20.94 | | I | C |
| | MOTA | 3551 | CG1 | VAL I | 54 | 38.791 | 4.820 | 78.352 | 1.00 11.51 | | Ī | C |
| | MOTA | 3552 | CG2 | VAL I | 54 | 38.453 | 2.385 | 78.975 | 1.00 17.89 | | I | C |
| | MOTA | 3553 | N | SER I | 55 | 39.278 | 6.374 | 81.258 | 1.00 33.89 | | I | N |
| | ATOM | 3554 | CA | SER I | 55 | 39.169 | 7.797 | 81.566 | 1.00 34.19 1.00 33.52 | | I I | C |
| 40 | ATOM | 3555 | C | SER I | 55 | 39.539 | 8.646 | 80.383 79.553 | 1.00 33.52 | | I I | Ö |
| | MOTA | 3556 | 0 | SER I | 55 | 40.396 | 8.279 8.161 | 82.724 | 1.00 37.31 | | Ī | č |
| | MOTA | 3557 | CB | SER I | 55 | $\frac{40.112}{40.101}$ | 9.570 | 82.724 | 1.00 53.86 | | Ī | ŏ |
| | MOTA | 3558 | OG | SER I GLY I | 55 56 | 38.880 | 9.774 | 80.267 | 1.00 28.58 | | Ī | N |
| 45 | MOTA | 3559 3560 | 'N CA | GLY I | 56 | 39.231 | 10.704 | 79.205 | 1.00 28.05 | | I | C |
| 45 | ATOM ATOM | 3561 | CA | GLY I | 56 | 38.958 | 10.276 | 77.774 | 1.00 29.97 | | I | С |
| | ATOM | 3562 | Ö | GLY I | 56 | 39.636 | 10.722 | 76.851 | 1.00 30.95 | | I | 0 |
| | ATOM | 3563 | N | CYS I | 57 | 37.958 | 9.430 | 77.564 | 1.00 27.62 | | I | N |
| | ATOM | 3564 | CA | CYS I | 57 | 37.678 | 8.988 | 76.196 | 1.00 24.77 | | I | С |
| 50 | MOTA | 3565 | C | CYS I | 57 | 36.192 | 9.169 | 75.867 | 1.00 26.27 | | I | C |
| | ATOM | 3566 | 0 | CYS I | 57 | 35.354 | 8.295 | 76.128 | 1.00 27.58 | | I | 0 |
| | MOTA | 3567 | CB | CYS I | 57 | 38.064 | 7.535 | 76.040 | 1.00 24.74 | | I | C |
| | MOTA | 3568 | SG | CYS I | 57 | 38.040 | 7.007 | 74.290 | 1.00 28.66 | | I | S |
| | MOTA | 3569 | N | SER I | 58 | 35.861 | 10.298 | 75.257 | 1.00 22.20 | | I | Ŋ |
| 55 | ATOM | 3570 | CA | SER I | 58 | 34.449 | 10.516 | 74.948 | 1.00 18.10 | | I | C |
| | MOTA | 3571 | С | SER I | 58 | 33.950 | 9.507 | 73.891 | 1.00 18.99 | | I | C |
| | ATOM | 3572 | 0 | SER I | 58 | 32.743 | 9.210 | 73.802 | 1.00 20.20 | | I | 0 |
| | MOTA | 3573 | СВ | SER I | 58 | 34.241 | 11.957 | 74.461 | 1.00 13.59 | | I | C |
| | MOTA | 3574 | OG | SER I | 58 | 35.149 | 12.274 | 73.404 | 1.00 17.58 | | I I | N |
| 60 | ATOM | 3575 | N | ALA I | 59 | 34.845 | 8.928 | 73.104 | 1.00 20.43 1.00 20.58 | | I | C |
| | ATOM | 3576 | CA | ALA I | 59 50 | 34.351 | 7.992 | 72.058 72.583 | 1.00 20.38 | | I | C |
| | ATOM | 3577 | C | ALA I | 59 | 33.723 | 6.699 | 72.583 | 1.00 23.25 | | Ī | Ö |
| | MOTA | 3578 | 0 | ALA I | 59 50 | 32.944 35.473 | 6.047 7.625 | 71.108 | 1.00 24.07 | | Ī | č |
| C.F | MOTA | 3579 | CB | ALA I ILE I | 59 60 | 34.084 | | 73.804 | 1.00 25.09 | | Ī | N |
| 65 | MOTA | 3580 3581 | N CA | ILE I | 60 | 33.563 | 5.064 | 74.404 | 1.00 25.81 | | I | Ĉ |
| | MOTA MOTA | 3582 | CA | ILE I | 60 | 32.326 | | 75.280 | 1.00 25.44 | | I | С |
| | MOTA | 3583 | Ö | ILE I | 60 | 31.719 | | 75.753 | 1.00 29.14 | | I | 0 |
| | MOTA | 3584 | | ILE I | | 34.693 | | 75.268 | 1.00 26.48 | | I | C |
| | | | | | | | | | | | | |

| | n | | | | | | | | | | | | |
|----|------|------|-------------|-------|----------|-------|-----|--------|--------|---------|------|--------|---|
| | ATOM | 3585 | CG1 | ILE I | 60 | 34.42 | 29 | 2.873 | 75.383 | 1.00 29 | | Γ | C |
| | ATOM | 3586 | | ILE I | 60 | 34.77 | 70 | 5.007 | 76.682 | 1.00 27 | .68 | I | C |
| | ATOM | 3587 | CD1 | ILE I | 60 | 34.78 | 38 | 2.139 | 74.124 | 1.00 35 | .86 | Ι | С |
| | ATOM | 3588 | N | GLU I | 61 | 31.93 | L6 | 6.504 | 75.486 | 1.00 27 | .58 | I, | N |
| 5 | ATOM | 3589 | | GLU I | 61 | 30.78 | 36 | 6.713 | 76.376 | 1.00 28 | 3.09 | I | C |
| J | ATOM | 3590 | | GLU I | 61 | 29.50 | | 6.014 | 75.949 | 1.00 23 | .64 | Ι | C |
| | ATOM | 3591 | | GLU I | 61 | 28.84 | | 5.387 | 76.747 | 1.00 22 | 2.27 | I | 0 |
| | ATOM | 3592 | | GLU I | 61 | 30.53 | | 8.216 | 76.576 | 1.00 28 | 3.67 | I | С |
| | MOTA | 3593 | | GLU I | 61 | 29.64 | | 8.435 | 77.799 | | 5.14 | I | С |
| 10 | ATOM | 3594 | CD | GLU I | 61 | 29.43 | | 9.895 | 78.121 | 1.00 79 | 3.31 | I | С |
| 10 | ATOM | 3595 | | GLU I | 61 | 30.4 | | 0.575 | 78.443 | | 7.35 | I | 0 |
| | | 3596 | | GLU I | 61 | 28.20 | | 0.350 | 78.034 | 1.00 78 | | I | 0 |
| | MOTA | | | LYS I | 62 | 29.1 | | 6.110 | 74.675 | | 2.10 | Ī | N |
| | MOTA | 3597 | N CA | LYS I | 62 | 27.9 | | 5.485 | 74.230 | | 1.59 | Ī | Ċ |
| | ATOM | 3598 | | LYS I | | 28.0 | | 3.960 | 74.460 | | 2.50 | Ī | Č |
| 15 | ATOM | 3599 | | | 62 62 | 27.0 | | 3.348 | 74.913 | | 5.76 | Ī | Õ |
| | ATOM | 3600 | O | LYS I | | 27.0 | | 5.788 | 72.749 | | 5.19 | I | Č |
| | MOTA | 3601 | CB | LYS I | 62 | | | 5.255 | 72.179 | | 3.62 | I | Č |
| | MOTA | 3602 | CG | LYS I | 62 | 26.4 | | | 70.789 | 1.00 40 | | Ī | Č |
| | ATOM | 3603 | CD | LYS I | | 26.2 | | 5.870 | 70.789 | 1.00 40 | | I | Č |
| 20 | ATOM | 3604 | CE | LYS I | 62 | 25.0 | | 5.242 | | 1.00 3 | | I | N |
| | MOTA | 3605 | NZ | LYS I | | 24.8 | | 5.985 | 68.770 | | | I | N |
| | MOTA | 3606 | N | THR I | | 29.1 | | 3.350 | 74.157 | 1.00 17 | 5.79 | I | C |
| | MOTA | 3607 | $^{\rm CA}$ | THR I | | 29.3 | | 1.914 | 74.390 | | | | C |
| | MOTA | 3608 | С | THR I | | 29.1 | | 1.594 | 75.880 | 1.00 19 | | I I | 0 |
| 25 | MOTA | 3609 | 0 | THR I | | 28.4 | | 0.633 | 76.237 | 1.00 18 | | | |
| | MOTA | 3610 | CB | THR I | | 30.7 | | 1.454 | 73.932 | 1.00 19 | | Ī | C |
| | ATOM | 3611 | OG1 | THR I | | 30.8 | | 1.607 | 72.498 | 1.00 24 | | I | 0 |
| | ATOM | 3612 | CG2 | THR I | | 30.9 | | -0.029 | 74.284 | 1.00 1 | | I | C |
| | MOTA | 3613 | N | GLN I | 64 | 29.6 | 66 | 2.414 | 76.786 | 1.00 18 | | I | N |
| 30 | MOTA | 3614 | CA | GLN I | 64 | 29.4 | | 2.123 | 78.195 | 1.00 1 | | I | C |
| | ATOM | 3615 | С | GLN I | 64 | 27.9 | | 2.127 | 78.570 | 1.00 1 | | I | C |
| | ATOM | 3616 | 0 | GLN I | 64 | 27.4 | | 1.301 | 79.334 | | 7.63 | I | 0 |
| | MOTA | 3617 | CB | GLN I | 64 | 30.1 | 94 | 3.123 | 79.104 | 1.00 1 | | I | C |
| | ATOM | 3618 | CG | GLN I | 64 | 31.7 | 12 | 3.131 | 78.912 | | 1.19 | I | C |
| 35 | ATOM | 3619 | CD | GLN I | 64 | 32.3 | 43 | 4.307 | 79.685 | 1.00 2 | 0.97 | I | С |
| | ATOM | 3620 | | GLN I | 64 | 31.6 | 56 | 5.290 | 79.958 | 1.00 2 | 6.32 | I | 0 |
| | ATOM | 3621 | NE2 | GLN I | 64 | 33.6 | 17 | 4.184 | 80.081 | 1.00 1 | | I | N |
| | MOTA | 3622 | N | ARG I | | 27.2 | 12 | 3.077 | 78.002 | 1.00 1 | 6.69 | I | N |
| | ATOM | 3623 | CA | ARG I | | 25.8 | | 3.242 | 78.268 | 1.00 1 | 8.05 | I | С |
| 40 | ATOM | 3624 | C | ARG I | | 24.9 | | 2.120 | 77.653 | 1.00 2 | 0.85 | I | C |
| 40 | ATOM | 3625 | Ö | ARG I | | 24.0 | | 1.620 | 78.264 | 1.00 2 | 1.77 | I | 0 |
| | ATOM | 3626 | ČВ | ARG I | | 25.3 | | 4.587 | 77.714 | 1.00 1 | 7.49 | I | C |
| | ATOM | 3627 | CG | ARG I | | 25.9 | | 5.731 | 78.482 | 1.00 2 | 7.25 | I | C |
| | ATOM | 3628 | CD | ARG I | | 25.5 | | 7.103 | 77.925 | 1.00 3 | 6.17 | I | C |
| 45 | MOTA | 3629 | NE | ARG I | | 26.0 | | 8.153 | 78.793 | 1.00 4 | 9.27 | I | N |
| 40 | MOTA | 3630 | CZ | ARG I | | 25.5 | | 8.457 | 79.994 | 1.00 4 | | I | C |
| | MOTA | 3631 | | ARG I | | 24.5 | | 7.800 | 80.475 | 1.00 3 | 0.90 | I | N |
| | ATOM | 3632 | | ARG 3 | | 26.1 | | 9.417 | 80.718 | 1.00 4 | | I | N |
| | ATOM | 3633 | N | MET] | | 25.3 | | 1.695 | 76.453 | 1.00 2 | | I | N |
| 50 | MOTA | 3634 | ČA | MET I | | 24.6 | | 0.574 | 75.849 | 1.00 1 | | I | C |
| 50 | | 3635 | CA | MET 3 | | 24.9 | | -0.730 | 76.616 | 1.00 1 | | I | C |
| | ATOM | 3636 | Ö | MET 3 | | 23.9 | | -1.524 | 76.829 | 1.00 1 | | I | 0 |
| | ATOM | | | | | 25.1 | | 0.430 | 74.388 | 1.00 1 | | Ī | Č |
| | ATOM | 3637 | CB | MET : | | 24.5 | | 1.557 | 73.502 | 1.00 2 | | Ī | Č |
| | ATOM | 3638 | CG | MET | | | | 1.443 | 71.840 | 1.00 2 | | Ī | s |
| 55 | MOTA | 3639 | SD | MET | | 25.3 | | 1.367 | 70.841 | 1.00 2 | | Ī | Č |
| | ATOM | 3640 | CE | MET : | | 23.8 | | | | 1.00 1 | | Ī | N |
| | ATOM | 3641 | N | LEU | | 26.1 | | -0.951 | 77.060 | 1.00 1 | | I | C |
| | MOTA | 3642 | CA | LEU : | | 26.4 | | -2.129 | 77.880 | | | | |
| | ATOM | 3643 | C | LEU : | | 25.6 | | -2.015 | 79.226 | 1.00 1 | | I | C |
| 60 | MOTA | 3644 | 0 | LEU : | | 25.1 | | -3.016 | 79.799 | 1.00 1 | | I | 0 |
| | MOTA | 3645 | CB | LEU : | | 27.9 | | -2.218 | 78.136 | 1.00 1 | | I | C |
| | MOTA | 3646 | CG | LEU : | | 28.7 | | -2.694 | 76.907 | 1.00 1 | | I | C |
| | MOTA | 3647 | | LEU : | | 30.2 | | -2.561 | 77.275 | 1.00 1 | 5.28 | I | C |
| | MOTA | 3648 | CD2 | LEU : | | 28.4 | | -4.176 | 76.515 | 1.00 1 | | I | C |
| 65 | MOTA | 3649 | N | SER : | | 25.5 | | -0.799 | 79.745 | 1.00 1 | | I | N |
| | ATOM | 3650 | CA | SER : | | 24.7 | | -0.628 | 80.994 | 1.00 1 | | I | C |
| | ATOM | 3651 | С | SER : | | 23.3 | | -1.021 | 80.848 | 1.00 1 | | I | C |
| | MOTA | 3652 | 0 | SER | | 22.6 | 556 | -1.463 | 81.806 | 1.00 2 | | I | 0 |
| | ATOM | 3653 | CB | SER | | 24.8 | | 0.834 | 81.481 | 1.00 1 | 5.42 | I | С |

| | ATOM | 3654 | OG | SER I | 68 | •• | 26.229 | 1.168 | 81.816 | 1.00 24.18 | | I | 0 |
|----|--------------|--------------|----------|----------------|----------|----|------------------|-------------------|------------------|--------------------------|---|--------|--------|
| | MOTA | 3655 | N | GLY I | 69 69 | | 22.788 21.422 | -0.863 -1.229 | 79.636 79.310 | 1.00 17.78 1.00 13.18 | | I | N C |
| | ATOM ATOM | 3656 3657 | CA C | GLY I | 69 | | 21.422 | -2.746 | 79.355 | 1.00 15.71 | | Ī | č |
| 5 | ATOM | 3658 | ŏ | GLY I | 69 | | 20.279 | -3.242 | 79.800 | 1.00 14.07 | | I | 0 |
| _ | MOTA | 3659 | N | PHE I | 70 | | 22.324 | -3.495 | 78.889 | 1.00 17.98 | | I | И |
| | MOTA | 3660 | CA | PHE I | 70 70 | | 22.265 22.523 | -4.948 -5.477 | 78.947 80.370 | 1.00 18.28 1.00 18.48 | | I | C C |
| | ATOM ATOM | 3661 3662 | C O | PHE I | 70 | | 22.034 | -6.564 | 80.757 | 1.00 18.81 | | Ī | ŏ |
| 10 | ATOM | 3663 | CB | PHE I | 70 | | 23.346 | -5.574 | 78.019 | 1.00 18.99 | | I | C |
| | MOTA | 3664 | CG | PHE I | 70 | | 22.947 | -5.624 | 76.570 | 1.00 19.17 | | I | C |
| | ATOM | 3665 | CD1 | PHE I | 70 | | 23.433 | -4.685 -6.634 | 75.683 76.115 | 1.00 13.86 1.00 14.02 | | I | C |
| | ATOM ATOM | 3666 3667 | | PHE I | 70 70 | | 22.121 23.086 | -4.746 | 74.297 | 1.00 15.78 | | Ī | č |
| 15 | ATOM | 3668 | CE2 | PHE I | 70 | | 21.757 | -6.719 | 74.732 | 1.00 21.48 | - | I | C |
| | MOTA | 3669 | CZ | PHE I | 70 | | 22.244 | -5.766 | 73.841 | 1.00 19.98 | | I | C |
| | MOTA | 3670 | N | CYS I | 71 | | 23.299 | -4.720 | 81.159 82.511 | 1.00 15.72 1.00 19.25 | | I | C N |
| | MOTA | 3671 | CA | CYS I | 71 71 | | 23.613 23.288 | -5.186 -4.039 | 83.511 | 1.00 19.23 | | Ï | Č |
| 20 | MOTA ATOM | 3672 3673 | C | CYS I | 71 | | 24.209 | -3.472 | 84.088 | 1.00 17.72 | | Ī | 0 |
| 20 | ATOM | 3674 | СВ | CYS I | 71 | | 25.118 | -5.443 | 82.612 | 1.00 17.63 | | I | C |
| | ATOM | 3675 | SG | CYS I | 71 | | 25.681 | -5.978 | 84.268 | 1.00 22.27 1.00 20.43 | | I I | s N |
| | ATOM | 3676 | N | PRO I | 72 72 | | 22.004 21.615 | -3.667 -2.570 | 83.656 84.563 | 1.00 20.43 | | I | C |
| 25 | ATOM ATOM | 3677 3678 | CA C | PRO I PRO I | 72 | | 21.849 | -2.796 | 86.063 | 1.00 18.35 | | Ī | Č |
| 20 | MOTA | 3679 | ŏ | PRO I | 72 | | 22.041 | -1.806 | 86.804 | 1.00 18.45 | | I | 0 |
| | MOTA | 3680 | CB | PRO I | | | 20.124 | -2.345 | 84.201 | 1.00 20.03 | | I | C |
| | ATOM | 3681 | CG | PRO I | | | 19.660 20.825 | -3.743 -4.260 | 83.874 83.006 | 1.00 22.09 1.00 22.41 | | I | C |
| 30 | ATOM ATOM | 3682 3683 | CD N | PRO I HIS I | | | 21.844 | -4.066 | 86.502 | 1.00 19.47 | | Ī | N |
| 30 | ATOM | 3684 | ČA | HIS I | | | 22.089 | -4.412 | 87.888 | 1.00 19.66 | | I | С |
| | ATOM | 3685 | C | HIS I | | | 23.381 | -5.238 | 87.946 | 1.00 21.68 | | I | C |
| | MOTA | 3686 | 0 | HIS I | | | 23.562 20.900 | -6.213 -5.199 | 87.207 88.485 | 1.00 25.46 1.00 20.83 | | I I | 0 |
| 25 | ATOM ATOM | 3687 3688 | CB CG | HIS I | | | 19.672 | -3.199 | 88.703 | 1.00 20.03 | | Ī | Č |
| 35 | ATOM | 3689 | | HIS I | | | 19.304 | -3.876 | 89.943 | 1.00 16.76 | | I | N |
| | ATOM | 3690 | | HIS I | 73 | | 18.770 | -3.846 | 87.820 | 1.00 24.20 | | Ĩ | C |
| | MOTA | 3691 | | HIS I | | | 18.222 | -3.109 | 89.811 | 1.00 16.41 1.00 15.39 | | I | C N |
| 10 | MOTA | 3692 | | HIS I | | | 17.878 24.275 | -3.082 -4.823 | 88.540 88.824 | 1.00 15.39 | | Ï | N |
| 40 | ATOM ATOM | 3693 3694 | N CA | LYS I | | | 25.558 | -5.460 | 88.935 | 1.00 21.35 | | I | C |
| | ATOM | 3695 | C | LYS I | | | 25.414 | -6.919 | 89.274 | 1.00 23.89 | | I | C |
| | MOTA | 3696 | 0 | LYS I | | | 24.528 | -7.310 | 90.044 | 1.00 22.28 | | I | 0 |
| 45 | MOTA | 3697 | CB CG | LYS I | | | 26.406 27.911 | -4.771 -5.064 | 90.030 89.908 | 1.00 22.82 1.00 21.50 | | I | C |
| 45 | MOTA MOTA | 3698 3699 | CD | LYS I | | | 28.751 | -4.501 | 91.096 | 1.00 16.86 | | Ī | С |
| | MOTA | 3700 | CE | LYS I | | | 28.597 | -5.307 | 92.383 | 1.00 15.58 | | I | C |
| | 'MOTA | 3701 | NZ | LYS I | | | 29.438 | -4.661 | 93.459 | 1.00 28.77 | | I | N |
| | ATOM | 3702 | N | VAL I | | | 26.291 26.315 | -7.728 -9.147 | 88.692 88.987 | 1.00 30.24 1.00 32.25 | | I | C N |
| 50 | MOTA MOTA | 3703 3704 | CA C | VAL I | | | 27.653 | -9.491 | 89.629 | 1.00 33.25 | | Ī | Č |
| | MOTA | 3705 | ŏ | VAL 3 | | | 28.590 | -8.668 | 89.633 | 1.00 36.67 | | I | 0 |
| | MOTA | 3706 | CB | VAL] | | | 26.106 | -9.983 | 87.715 | 1.00 31.71 | | I | C |
| | MOTA | 3707 | | VAL 3 | | | 24.737 | -9.626 -9.701 | 87.122 86.667 | 1.00 30.96 1.00 37.27 | | I | C |
| 55 | ATOM ATOM | 3708 3709 | N N | VAL I SER I | | | 27.251 27.742 | | 90.227 | 1.00 37.27 | | Ī | N |
| | ATOM | 3710 | CA | SER J | | | 29.010 | -11.098 | 90.839 | 1.00 43.38 | | I | C |
| | ATOM | 3711 | C | SER I | | | 30.110 | -11.307 | 89.793 | 1.00 45.20 | | I | C |
| | MOTA | 3712 | 0 | SER : | | | | -12.056 | 88.832 | 1.00 41.71 | | I | C 0 |
| 60 | MOTA | 3713 | CB | SER : | | | | -12.402 -12.787 | 91.626 92.120 | 1.00 45.35 1.00 51.24 | | I | Ö |
| | ATOM ATOM | 3714 3715 | OG N | SER I | | | | -10.652 | 89.982 | 1.00 49.67 | | Ī | N |
| | ATOM | 3716 | CA | ALA : | | | 32.375 | -10.766 | 89.048 | 1.00 54.47 | | I | С |
| | MOTA | 3717 | C | ALA : | 77 | | 32.943 | -12.175 | 89.034 | 1.00 57.42 | | I | C |
| 65 | ATOM | 3718 | 0 | ALA : | | | | -12.653 | 88.003 89.414 | 1.00 59.50 1.00 51.64 | | I | 0 |
| | ATOM ATOM | 3719 3720 | CB N | ALA : | | | 33.478 32.895 | -9.766 -12.843 | 90.179 | 1.00 51.04 | | Ī | N |
| | ATOM | 3721 | CA | GLY : | | | 33.412 | -14.198 | 90.239 | 1.00 62.69 | | I | C |
| | ATOM | 3722 | C | GLY : | 78 | | 34.882 | -14.206 | 89.849 | 1.00 63.55 | | I | С |

| | ATOM | 3723 | O GLY I | | 35 563 | -13.090 | 90.291 | 1.00 63.76 | I | 0 |
|----------------|--------------|--------------|--------------------|------|------------------|--------------------|------------------|--------------------------|---|--------|
| | ATOM | 3724 | N SER I | | | -16.327 | 92.121 | 1.00 67.81 | I | N |
| | ATOM | 3725 | CA SER I | | | -16.933 | 92.348 | 1.00 65.14 | I | C |
| | MOTA | 3726 | C SER I | | | -16.541 | 91.309 | 1.00 61.18 | I | C |
| [.] 5 | MOTA | 3727 | O SER I | | | -16.954 | 91.421 | 1.00 60.41 | I | 0 |
| | ATOM | 3728 | CB SER I | | | -18.457 | 92.368 | 1.00 65.70 1.00 69.36 | I | C O |
| | MOTA | 3729 | OG SER I | | | -18.891 -15.751 | 93.492 90.310 | 1.00 69.36 1.00 56.70 | I | N |
| | MOTA | 3730 | N SER I | | | -15.344 | 89.249 | 1.00 51.54 | Î | Ĉ |
| 10 | ATOM ATOM | 3731 3732 | CA SER I | | | -14.090 | 89.610 | 1.00 47.03 | Ī | č |
| 10 | ATOM | 3733 | O SER I | | | -12.987 | 89.727 | 1.00 44.40 | I | 0 |
| | MOTA | 3734 | CB SER I | | | -15.117 | 87.966 | 1.00 52.88 | I | C |
| | MOTA | 3735 | OG SER I | 82 | | -14.947 | 86.868 | 1.00 62.13 | I | 0 |
| | MOTA | 3736 | N LEU I | | 44.992 | | 89.782 | 1.00 40.85 | I | N |
| 15 | MOTA | 3737 | CA LEU I | | 45.839 | | 90.182 | 1.00 33.26 | I | C |
| | ATOM | 3738 | C LEU | | 45.835 | -11.917 | 89.264 89.748 | 1.00 32.94 1.00 30.66 | I | Ö |
| | ATOM | 3739 | O LEU I | | 45.828 47.287 | | 90.310 | 1.00 30.00 | ī | č |
| | ATOM | 3740 3741 | CB LEU I | | 48.279 | | 90.838 | 1.00 27.09 | Ī | č |
| 20 | ATOM ATOM | 3742 | CD1 LEU | | 47.939 | | 92.295 | 1.00 12.16 | I | C |
| 20 | ATOM | 3743 | CD2 LEU | | 49.691 | | 90.750 | 1.00 24.42 | I | C |
| | ATOM | 3744 | N HIS | 84 | 45.872 | -12.145 | 87.957 | 1.00 29.82 | I | N |
| | ATOM | 3745 | CA HIS | | 45.974 | | 86.983 | 1.00 29.54 | Ī | C |
| | MOTA | 3746 | C HIS | | 44.628 | | 86.425 | 1.00 29.73 | I | C |
| 25 | ATOM | 3747 | O HIS | | 44.592 | -9.730 -11.516 | 85.525 85.820 | 1.00 25.19 1.00 26.32 | I | C O |
| | ATOM | 3748 | CB HIS CG HIS | | 46.850 48.157 | | 86.250 | 1.00 28.45 | Ī | č |
| | ATOM | 3749 3750 | CG HIS I | | 49.148 | | 86.849 | 1.00 29.88 | Ī | N |
| | ATOM ATOM | 3751 | CD2 HIS | | | -13.377 | 86.169 | 1.00 24.74 | I | C |
| 30 | ATOM | 3752 | CE1 HIS | | | -12.144 | 87.123 | 1.00 30.46 | I | С |
| 00 | ATOM | 3753 | NE2 HIS | | | -13.372 | 86.721 | 1.00 21.40 | I | N |
| | MOTA | 3754 | N VAL | | 43.536 | | 86.978 | 1.00 32.07 | Ī | N |
| • | MOTA | 3755 | CA VAL | | 42.202 | | 86.471 | 1.00 32.06 | I | C |
| | ATOM | 3756 | C VAL | | 41.928 | | 86.189 85.194 | 1.00 33.84 1.00 36.05 | I | C O |
| 35 | ATOM | 3757 | O VAL | | 41.269 41.112 | | 87.405 | 1.00 33.38 | Ī | · Č |
| | MOTA | 3758 3759 | CB VAL CG1 VAL | | 41.122 | | 88.753 | 1.00 33.30 | Ī | č |
| | MOTA MOTA | 3760 | CG2 VAL | | 39.765 | | 86.751 | 1.00 37.69 | I | C |
| | ATOM | 3761 | N ARG | | 42.424 | | 87.022 | 1.00 32.54 | I | N |
| 40 | ATOM | 3762 | CA ARG | | 42.181 | -6.974 | 86.794 | 1.00 31.61 | I | C |
| | MOTA | 3763 | C ARG | | 43.401 | | 86.290 | 1.00 31.91 | I | C |
| | MOTA | 3764 | O ARG | | 43.435 | | 86.319 | 1.00 35.23 | I | 0 |
| | ATOM | 3765 | CB ARG | | 41.586 | | 88.074 88.217 | 1.00 28.40 1.00 41.94 | Ī | C |
| 45 | MOTA | 3766 | CG ARG CD ARG | | 40.089 39.461 | | 89.534 | 1.00 41.34 | Ī | Č |
| 45 | ATOM ATOM | 3767 3768 | CD ARG NE ARG | | 39.546 | | 90.565 | 1.00 63.98 | Ī | N |
| | ATOM | 3769 | CZ ARG | | 38.731 | | 90.654 | 1.00 66.04 | I | C |
| | MOTA | 3770 | NH1 ARG | | 37.746 | | 89.784 | 1.00 52.07 | I | N |
| | MOTA | 3771 | NH2 ARG | | 38.896 | | 91.647 | 1.00 62.26 | I | N |
| 50 | MOTA | 3772 | N ASP | | 44.409 | | 85.790 | 1.00 30.34 | Ī | N |
| | ATOM | 3773 | CA ASP | | 45.582 | | 85.271 | 1.00 32.40 1.00 31.30 | I | C C |
| | ATOM | 3774 | C ASP | | 45.118 | | 83.964 83.192 | 1.00 31.30 | I | Ö |
| | ATOM | 3775 | O ASP CB ASP | | 44.441 46.690 | | 84.879 | 1.00 34.02 | Ī | č |
| 55 | ATOM ATOM | 3776 3777 | CB ASP CG ASP | | 47.463 | | 86.086 | 1.00 38.19 | Ī | Č |
| 55 | ATOM | 3778 | OD1 ASP | | 47.145 | | 87.260 | 1.00 32.90 | I | 0 |
| | ATOM | 3779 | OD2 ASP | | 48.406 | | 85.741 | 1.00 32.57 | I | 0 |
| | MOTA | 3780 | N THR | | 45.516 | | 83.687 | 1.00 30.86 | Ī | N |
| | MOTA | 3781 | CA THR | I 88 | 45.063 | | 82.443 | 1.00 31.20 | I | C |
| 60 | MOTA | 3782 | C THR | | 46.075 | | 81.321 | 1.00 31.74 | I | C 0 |
| | ATOM | 3783 | O THR | | 46.942 | | 81.058 82.703 | 1.00 33.75 1.00 29.81 | I | G |
| | ATOM | 3784 | CB THR | | 44.822 46.02 | | 82.703 | 1.00 29.81 | I | Ö |
| | ATOM ATOM | 3785 3786 | OG1 THR CG2 THR | | 43.76 | | 83.782 | 1.00 24.42 | Ï | č |
| 65 | ATOM | 3787 | N ALA | | 45.968 | | 80.639 | 1.00 31.60 | I | N |
| 00 | ATOM | 3788 | CA ALA | | 46.95 | 5 -5.362 | 79.608 | 1.00 30.00 | I | C |
| | ATOM | 3789 | C ALA | | 46.448 | 3 -5.308 | 78.192 | 1.00 29.68 | Ī | |
| | ATOM | 3790 | O ALA | I 89 | 47.20 | | 77.282 | 1.00 32.56 | I | |
| | ATOM | 3791 | CB ALA | I 89 | 47.564 | 4 -6.708 | 79.859 | 1.00 35.66 | I | С |

| | n mes | | | ** | 0.0 | 45.203 | -4.897 | 77.975 | 1.00 26.67 | I | N |
|----|--------------|--------------|----------|---------|----------|-----------------|------------------|------------------|--------------------------|----|---|
| | MOTA | 3792 | N | ILE I | 90 | 45.203 | -4.930 | 76.618 | 1.00 20.07 | Ī | Ĉ |
| | MOTA | 3793 | CA | ILE I | 90 90 | 44.399 | -3.493 | 76.191 | 1.00 20.02 | Ī | Ċ |
| | ATOM | 3794 | C | ILE I | 90 | 43.796 | -2.739 | 76.949 | 1.00 18.80 | Ī | ō |
| _ | MOTA | 3795 3796 | O CB | ILE I | 90 | 43.309 | -5.690 | 76.590 | 1.00 22.56 | I | C |
| 5 | ATOM | 3790 3797 | CG1 | ILE I | 90 | 43.439 | -7.060 | 77.251 | 1.00 27.82 | I | C |
| | ATOM | 3798 | CG2 | ILE I | 90 | 42.780 | -5.835 | 75.178 | 1.00 20.25 | I | С |
| | ATOM ATOM | 3799 | | ILE I | 90 | 44.554 | -7.915 | 76.695 | 1.00 23.97 | I | С |
| | ATOM | 3800 | N | GLU I | 91 | 44.802 | -3.115 | 74.992 | 1.00 22.48 | I | N |
| 10 | ATOM | 3801 | CA | GLU I | 91 | 44.501 | -1.768 | 74.513 | 1.00 25.02 | I | С |
| 10 | ATOM | 3802 | C | GLU I | 91 | 42.983 | -1.709 | 74.241 | 1.00 25.25 | I | С |
| | ATOM | 3803 | ŏ | GLU I | 91 | 42.369 | -2.675 | 73.785 | 1.00 24.40 | I | 0 |
| | ATOM | 3804 | ČВ | GLU I | | 45.255 | -1.470 | 73.201 | 1.00 26.65 | I | C |
| | ATOM | 3805 | ĊĠ | GLU I | 91 | 46.761 | -1.457 | 73.383 | 1.00 43.52 | I | С |
| 15 | ATOM | 3806 | CD | GLU I | | 47.501 | -1.542 | 72.054 | 1.00 66.85 | I | C |
| | MOTA | 3807 | | GLU I | | 48.725 | -1.840 | 72.074 | 1.00 71.43 | I | 0 |
| | ATOM | 3808 | OE2 | GLU I | 91 | 46.853 | -1.312 | 70.997 | 1.00 76.33 | I | 0 |
| | ATOM | 3809 | N | VAL I | | 42.374 | -0.559 | 74.508 | 1.00 20.39 | I | N |
| | ATOM | 3810 | CA | VAL I | 92 | 40.939 | -0.475 | 74.300 | 1.00 22.52 | Ī | C |
| 20 | ATOM | 3811 | С | VAL I | 92 | 40.523 | -0.874 | 72.888 | 1.00 24.09 | I | C |
| | ATOM | 3812 | 0 | VAL I | | 39.571 | -1.603 | 72.701 | 1.00 22.60 | I | 0 |
| | MOTA | 3813 | CB | VAL I | | 40.428 | 0.925 | 74.574 | 1.00 24.93 | I | C |
| | MOTA | 3814 | | VAL I | | 38.923 | 0.968 | 74.198 | 1.00 23.93 | Į | C |
| | MOTA | 3815 | CG2 | VAL I | | 40.622 | 1.268 | 76.076 | 1.00 29.40 | I | И |
| 25 | MOTA | 3816 | N | ALA I | | 41.241 | -0.393 | 71.889 | 1.00 23.14 | I | C |
| | MOTA | 3817 | CA | ALA I | | 40.901 | -0.747 | 70.521 | 1.00 20.90 1.00 21.97 | Ī | C |
| | MOTA | 3818 | C | ALA I | | 40.853 | -2.249 | 70.320 69.631 | 1.00 21.97 | Ī | Ö |
| | MOTA | 3819 | 0 | ALA I | | 39.949 | -2.781 | 69.561 | 1.00 22.74 | Ī | č |
| | MOTA | 3820 | CB | ALA I | | 41.903 | -0.116 -2.953 | 70.883 | 1.00 20.31 | Ī | N |
| 30 | ATOM | 3821 | N | ALA I | | 41.832 | -2.933 -4.420 | 70.728 | 1.00 20.31 | Ĩ | Ĉ |
| | ATOM | 3822 | CA | ALA I | | 41.883 | -4.420 -5.113 | 70.728 | 1.00 21.47 | Ī | č |
| | ATOM | 3823 | C | ALA I | | 40.764 40.140 | -6.098 | 70.998 | 1.00 21.47 | Ī. | ŏ |
| | ATOM | 3824 | 0 | ALA I | | 43.276 | -4.974 | 71.187 | 1.00 23.67 | I | Č |
| | ATOM | 3825 | CB | ALA I | | 40.483 | -4.584 | 72.672 | 1.00 19.72 | Ī | Ŋ |
| 35 | ATOM | 3826 | N | PHE I | | 39.426 | -5.132 | 73.479 | 1.00 19.20 | I | C |
| | MOTA | 3827 | CA | | | 38.072 | -5.000 | 72.750 | 1.00 20.71 | I | C |
| | ATOM | 3828 | C | PHE I | | 37.284 | -5.941 | 72.715 | 1.00 18.83 | I | 0 |
| | ATOM | 3829 | O | PHE I | | 39.352 | -4.371 | 74.805 | 1.00 17.19 | I | C |
| 40 | MOTA | 3830 3831 | CB CG | PHE I | | 38.253 | -4.836 | 75.695 | 1.00 18.73 | I | C |
| 40 | MOTA | 3832 | | L PHE 3 | | 38.509 | -5.739 | 76.707 | 1.00 19.09 | I | С |
| | ATOM ATOM | 3833 | | PHE | | 36.939 | -4.365 | 75.517 | 1.00 28.45 | I | C |
| | ATOM | 3834 | | L PHE | | 37.475 | -6.189 | 77.554 | 1.00 24.24 | I | С |
| | MOTA | 3835 | | PHE | | 35.914 | -4.798 | 76.346 | 1.00 28.64 | I | С |
| 45 | MOTA | 3836 | CZ | PHE | | 36.172 | -5.706 | 77.360 | 1.00 28.20 | I | C |
| 40 | MOTA | 3837 | N | VAL : | | 37.814 | -3.817 | 72.186 | 1.00 21.23 | I | N |
| | MOTA | 3838 | CA | VAL | | 36.534 | -3.564 | 71.499 | 1.00 22.02 | I | C |
| | MOTA | 3839 | C | VAL 3 | I 96 | 36.412 | -4.391 | 70.191 | 1.00 22.65 | I | C |
| | MOTA | 3840 | Ō | | I 96 | 35.358 | -4.954 | 69.862 | 1.00 22.48 | I | 0 |
| 50 | MOTA | 3841 | СВ | | I 96 | 36.354 | -2.048 | 71.208 | 1.00 22.55 | I | C |
| | ATOM | 3842 | CG: | 1 VAL | I 96 | 35.086 | -1.833 | 70.313 | 1.00 18.24 | Ī | C |
| | MOTA | 3843 | CG | 2 VAL 3 | I 96 | 36.164 | -1.327 | 72.526 | 1.00 23.04 | Ī | C |
| | MOTA | 3844 | N | ALA : | I 97 | 37.506 | -4.495 | 69.452 | 1.00 25.04 | Ī | И |
| | MOTA | 3845 | CA | ALA : | | 37.467 | -5.306 | 68.235 | 1.00 26.44 | Ī | C |
| 55 | ATOM | 3846 | C | ALA : | I 97 | 37.132 | -6.762 | 68.567 | 1.00 22.96 | I | C |
| | MOTA | 3847 | 0 | | I 97 | 36.353 | -7.388 | 67.886 | 1.00 24.45 | I | |
| | MOTA | 3848 | CB | ALA | I 97 | 38.807 | -5.233 | 67.515 | 1.00 31.87 | Ī | |
| | MOTA | 3849 | N | ASP | I 98 | 37.709 | -7.303 | 69.627 | 1.00 23.71 | Ī | |
| | ATOM | 3850 | ca | | | 37.425 | -8.696 | 70.050 | 1.00 23.00 | Ī | |
| 60 | ATOM | 3851 | C | ASP | | 35.979 | -8.812 | 70.558 | 1.00 24.40 | I | |
| | ATOM | 3852 | 0 | ASP | I 98 | 35.283 | -9.795 | 70.294 | 1.00 24.30 | I | 0 |
| | ATOM | 3853 | СВ | | | 38.382 | -9.092 | 71.180 | 1.00 19.69 | I | C |
| | MOTA | 3854 | | | | 38.094 | -10.465 | 71.749 | 1.00 23.36 | I | C |
| | ATOM | 3855 | | 1 ASP | | 38.602 | | 71.271 | 1.00 32.56 | I | |
| 65 | ATOM | 3856 | | 2 ASP | | 37.296 | | | 1.00 25.79 | I | |
| | MOTA | 3857 | | LEU | | 35.540 | -7.819 | | 1.00 25.64 | I | |
| | MOTA | 3858 | CA | | | 34.158 | | | 1.00 23.64 | I | |
| | ATOM | 3859 | | LEU | | 33.254 | | | | I | |
| | ATOM | 3860 | 0 | LEU | I 99 | 32.302 | -8.681 | 70.575 | 1.00 21.05 | Т | U |

| | ATOM ATOM ATOM | 3861 3862 3863 | CB LEU I 99 CG LEU I 99 CD1 LEU I 99 | 33.832 -6.556 72.655 1.00 26.66 32.389 -6.402 73.163 1.00 20.95 31.978 -7.628 73.981 1.00 13.88 32.325 -5.070 73.966 1.00 24.83 | I I I | С С С |
|----|------------------------------|------------------------------|---|--|-------------|------------------|
| 5 | ATOM ATOM ATOM ATOM | 3864 3865 3866 3867 | CD2 LEU I 99 N LEU I 100 CA LEU I 100 C LEU I 100 | 33.545 -7.065 69.628 1.00 25.95 32.711 -6.993 68.426 1.00 28.26 32.627 -8.366 67.732 1.00 29.60 | I I I | С С И |
| 10 | ATOM ATOM ATOM ATOM | 3868 3869 3870 3871 | O LEU I 100 CB LEU I 100 CG LEU I 100 CD1 LEU I 100 | 31.560 -8.810 67.305 1.00 29.23 33.273 -5.928 67.452 1.00 30.11 32.650 -5.886 66.044 1.00 27.15 31.135 -5.727 66.148 1.00 31.05 | I I I | 0 0 0 |
| 15 | MOTA ATOM ATOM ATOM | 3872 3873 3874 3875 | CD2 LEU I 100 N LEU I 101 CA LEU I 101 C LEU I 101 | 33.281 -4.740 65.254 1.00 26.52 33.745 -9.063 67.675 1.00 29.37 33.759 -10.388 67.038 1.00 29.29 32.817 -11.370 67.738 1.00 27.17 | . I I | С И С |
| 10 | ATOM ATOM ATOM | 3876 3877 3878 | O LEU I 101 CB LEU I 101 CG LEU I 101 | 32.059 -12.118 67.095 1.00 28.05 35.207 -10.893 67.069 1.00 28.28 35.600 -12.250 66.508 1.00 32.38 37.152 -12.263 66.541 1.00 49.76 | I I I | 0 0 0 |
| 20 | ATOM ATOM ATOM ATOM | 3879 3880 3881 3882 | CD1 LEU I 101 CD2 LEU I 101 N HIS I 102 CA HIS I 102 | 35.018 -13.410 67.313 1.00 35.45 32.870 -11.373 69.071 1.00 26.61 32.034 -12.251 69.877 1.00 27.47 | I I I | C N C |
| 25 | ATOM ATOM ATOM ATOM | 3883 3884 3885 3886 | C HIS I 102 O HIS I 102 CB HIS I 102 CG HIS I 102 | 30.583 -11.798 69.756 1.00 29.67 29.681 -12.633 69.610 1.00 31.47 32.512 -12.240 71.343 1.00 24.82 33.836 -12.910 71.517 1.00 31.90 | I I I | 0000 |
| | ATOM ATOM ATOM | 3887 3888 3889 | ND1 HIS I 102 CD2 HIS I 102 CE1 HIS I 102 | 34.018 -14.251 71.250 1.00 35.56 35.057 -12.422 71.843 1.00 30.43 35.291 -14.560 71.396 1.00 33.85 | I I I | N C C N |
| 30 | ATOM ATOM ATOM ATOM | 3890 3891 3892 3893 | NE2 HIS I 102 N LEU I 103 CA LEU I 103 C LEU I 103 | 35.943 -13.472 71.756 1.00 40.02 30.337 -10.488 69.801 1.00 25.34 28.934 -10.065 69.640 1.00 23.49 28.346 -10.471 68.259 1.00 25.13 | I I E | C C |
| 35 | MOTA MOTA MOTA | 3894 3895 3896 | O LEU I 103 CB LEU I 103 CG LEU I 103 CD1 LEU I 103 | 27.187 -10.905 68.172 1.00 25.31 28.767 -8.550 69.831 1.00 21.97 29.020 -8.116 71.296 1.00 26.35 28.850 -6.663 71.451 1.00 19.33 | I I I | 0 0 0 |
| 40 | ATOM ATOM ATOM ATOM | 3897 3898 3899 3900 | CD2 LEU I 103 N LYS I 104 CA LYS I 104 | 28.028 -8.793 72.252 1.00 16.98 29.139 -10.363 67.198 1.00 24.74 28.632 -10.737 65.869 1.00 26.53 | I I | С И С |
| | MOTA MOTA MOTA MOTA | 3901 3902 3903 3904 | C LYS I 104 O LYS I 104 CB LYS I 104 CG LYS I 104 | 28.329 -12.220 65.811 1.00 27.50 27.366 -12.627 65.208 1.00 28.46 29.625 -10.357 64.783 1.00 22.88 29.587 -8.914 64.413 1.00 31.89 | I I I | С О С |
| 45 | ATOM ATOM ATOM | 3905 3906 3907 | CD LYS I 104 CE LYS I 104 NZ LYS I 104 | 30.631 -8.717 63.344 1.00 32.33 30.925 -7.279 63.115 1.00 59.68 32.076 -7.164 62.142 1.00 68.07 | I I | И С С |
| 50 | MOTA MOTA MOTA MOTA | 3908 3909 3910 3911 | N ALA I 105 CA ALA I 105 C ALA I 105 O ALA I 105 | 29.133 -13.023 66.479 1.00 29.46 28.882 -14.450 66.534 1.00 34.23 27.563 -14.703 67.275 1.00 37.21 26.663 -15.418 66.770 1.00 39.76 | I I I | О С И |
| | MOTA MOTA MOTA | 3912 3913 3914 | CB ALA I 105 N LEU I 106 CA LEU I 106 | 30.064 -15.163 67.232 1.00 32.11 27.411 -14.122 68.470 1.00 39.89 26.165 -14.309 69.230 1.00 38.09 | I I I | N C |
| 55 | MOTA MOTA MOTA MOTA | 3915 3916 3917 3918 | C LEU I 106 O LEU I 106 CB LEU I 106 CG LEU I 106 | 24.938 -13.890 68.408 1.00 37.88 23.913 -14.550 68.431 1.00 33.66 26.194 -13.477 70.530 1.00 36.52 24.863 -13.456 71.276 1.00 42.06 | I I I | 0000 |
| 60 | MOTA MOTA MOTA | 3919 3920 3921 | CD1 LEU I 106 CD2 LEU I 106 N PHE I 107 | 24.583 -14.853 71.860 1.00 38.67 24.917 -12.412 72.412 1.00 45.46 25.064 -12.790 67.683 1.00 38.60 | I I I | C C |
| 65 | ATOM ATOM ATOM ATOM | 3922 3923 3924 3925 | CA PHE I 107 C PHE I 107 O PHE I 107 CB PHE I 107 | 23.973 -12.279 66.867 1.00 40.37 23.618 -13.276 65.764 1.00 43.78 22.436 -13.549 65.529 1.00 44.25 24.365 -10.956 66.236 1.00 37.22 | I I I | C C C |
| 30 | ATOM ATOM ATOM ATOM | 3926 3927 3928 3929 | CG PHE I 107 CD1 PHE I 107 CD2 PHE I 107 | 23.271 -10.311 65.429 1.00 36.27 22.198 -9.699 66.048 1.00 46.75 23.322 -10.317 64.052 1.00 36.68 21.186 -9.098 65.296 1.00 35.59 | I I I | 0000 |
| | A I OII | 7223 | CHI 1111 1 107 | | | |

| | MOTA | 3930 | CE2 | PHE : | 107 | 22 | .320 | _9 | .717 | 63. | 299 | 1.00 | | | I | C |
|------|------|------|------------|-------|-------|-----|-------|------|----------------|---|-------|------|-------|-------|--------------|-----|
| | ATOM | 3931 | CZ | PHE : | | | .253 | | .109 | 63. | 923 | 1.00 | 39. | .35 | I | C |
| | ATOM | 3932 | N | ALA : | | | | | .786 | 65. | 075 | 1.00 | | | I | N |
| | ATOM | 3933 | CA | ALA : | 108 | | | | 1.758 | | 993 | 1.00 | 52. | .09 | I | С |
| = | ATOM | 3934 | C | ALA : | 108 | | | | .034 | | 566 | 1.00 | | | I | С |
| 5 | | | | ALA : | | | | | 5.540 | | 031 | 1.00 | | | Ī | Ö |
| | ATOM | 3935 | 0 | | | | | | 5.076 | | 280 | 1.00 | | | Ī | č |
| | ATOM | 3936 | CB | ALA | | | | | | | 659 | 1.00 | | | Ī | N |
| | ATOM | 3937 | N | ALA : | | | | | 5.543 | | | 1.00 | | | Ï | C |
| | MOTA | 3938 | CA | ALA : | | | | | 7.732 | | 338 | | | | I | C |
| 10 | ATOM | 3939 | C | ALA : | | | | | 7.549 | | 929 | 1.00 | | | | |
| | MOTA | 3940 | 0 | ALA : | | | | | 5.521 | | 672 | 1.00 | | | I | 0 |
| | MOTA | 3941 | CB | ALA : | I 109 | | | | 3.097 | | 470 | 1.00 | | | I | C |
| | MOTA | 3942 | OXT | ALA | I 109 | 22 | .003 | -18 | 3.464 | 67. | 674 | 1.00 | 70 | .12 | I | 0 |
| | TER | 3943 | | ALA | I 109 | | | | | | | | | | | |
| 15 | MOTA | 3944 | 04 | OAC | | 18 | 3.217 | 2: | 2.918 | 90. | 161 | 1.00 | 51 | .17 | S | 0 |
| .0 | ATOM | 3945 | Č2 | OAC | | | .505 | | L.950 | 89. | 542 | 1.00 | 51 | .08 | S | С |
| | ATOM | 3946 | 03 | OAC | | | 3.384 | | L.569 | | 864 | 1.00 | 56 | . 88 | S | 0 |
| | ATOM | 3947 | C1 | OAC | | | 3.305 | | 1.429 | | 360 | 1.00 | 58 | . 69 | S | С |
| | TER | 3948 | Ç.L | OAC | | | | , 4. | | • | | | | | | |
| 00 | | | 77 NT | | z 1 | 26 | 5.522 | | 5.968 | 101 | 166 | 1.00 | 26 | 39 | \mathbf{z} | zn |
| 20 | MOTA | 3949 | ZN | | | | .447 | _ | 9.432 | | 331 | 1.00 | | | z | ZN |
| | MOTA | 3950 | ZN | | | | | | 0.777 | | 988 | 1.00 | | | z | ZN |
| | MOTA | 3951 | ΣN | | Z 3 | ∠(|).593 | • | 3.777 | 05. | . 500 | 1.00 | ' ' | .)) | <i>د</i> ا | 211 |
| | TER | 3952 | _ | | Z 3 | 0.4 | | | | 0.0 | 000 | 1 00 | 0 | 40 | Ta7 | 0 |
| | MOTA | 3953 | 0 | HOH | | | 3.273 | | 1.562 | | 929 | 1.00 | | .42 | W | 0 |
| 25 | MOTA | 3954 | 0 | HOH | | | 3.494 | | 3.183 | | 025 | 1.00 | | | M | 0 |
| | MOTA | 3955 | 0 | HOH | | _ | 0.63 | | 6.714 | | .029 | 1.00 | | .14 | M | 0 |
| | MOTA | 3956 | 0 | HOH | | | 3.09 | | 6.849 | | | 1.00 | | | M | 0 |
| | MOTA | 3957 | 0 | HOH | W 7 | 8 | 3.093 | | 3.904 | | | 1.00 | | | W | 0 |
| | ATOM | 3958 | 0 | HOH | 8 W | 18 | 3.32 | 9 1 | 5.295 | 86. | .054 | 1.00 | | | W | 0 |
| 30 | ATOM | 3959 | 0 | HOH | W 9 | 1: | L.64: | 3 1 | 7.561 | 91. | 629 | 1.00 | 19 | .27 | W | 0 |
| • | ATOM | 3960 | Ö | HOH | | 24 | 1.50 | 3 | 1.519 | 109 | .138 | 1.00 | 13 | .78 | W | 0 |
| | ATOM | 3961 | Ŏ | НОН | | | 3.56 | | 9.514 | | .581 | 1.00 | 11 | .36 | W | 0 |
| | ATOM | 3962 | Ö | HOH | | | 1.31 | | 0.426 | | .254 | 1.00 | 21 | .71 | W | 0 |
| | ATOM | 3963 | ŏ | HOH | | | 3.62 | | 9.471 | | .511 | 1.00 | 7 | .65 | W | 0 |
| O.E. | | 3964 | ŏ | НОН | | | 3.27 | | 6.451 | | .834 | 1.00 | | | W | 0 |
| 35 | ATOM | | | | | | 3.23 | | 6.147 | | | 1.00 | | | W | Ō |
| | ATOM | 3965 | 0 | HOH | | | 6.16 | _ | 0.147 0.823 | | | 1.00 | | | W | ŏ |
| | ATOM | 3966 | 0 | HOH | | | | | 2.988 | | | 1.00 | 17 | 97 | W | ŏ |
| | MOTA | 3967 | 0 | HOH | | | 7.91 | | | | .874 | 1.00 | | | W | Ö |
| | MOTA | 3968 | 0 | HOH | | | 2.75 | | 9.187 | | | 1.00 | | | W | ő |
| 40 | MOTA | 3969 | 0 | HOH | | | 5.44 | | 0.063 | | .133 | | | | | Ö |
| | MOTA | 3970 | 0 | HOH | | | 7.62 | | 2.548 | | .823 | 1.00 | | | W | |
| | MOTA | 3971 | | HOH | | | 8.77 | | 2.300 | | .542 | 1.00 | | | W | 0 |
| | MOTA | 3972 | 0 | HOH | | | 0.03 | | 1.543 | | .170 | 1.00 | | | M | 0 |
| | MOTA | 3973 | 0 | HOH | W 24 | | 5.81 | | 0.831 | | .674 | 1.00 | | | M | 0 |
| 45 | MOTA | 3974 | О | HOH | W 25 | | 0.38 | | 7.369 | | .168 | 1.00 | | | M | 0 |
| | ATOM | 3975 | 0 | HOH | W 26 | 3 | 0.61 | 12 | 1.516 | 90 | .986 | 1.00 | 24 | .22 | W | 0 |
| | MOTA | 3976 | 0 | HOH | W 27 | 1 | 6.02 | 6 3 | 0.411 | | .826 | | | | W | 0 |
| | ATOM | 3977 | | HOH | | 3 | 9.58 | 6 - | 2.015 | 82 | .847 | 1.00 | | | W | 0 |
| | ATOM | 3978 | | HOH | | 2 | 2.16 | 5 - | 7.013 | 84 | .963 | 1.00 | 21 | .19 | W | 0 |
| 50 | ATOM | 3979 | | HOH | | | 1.83 | | 1.471 | . 72 | .582 | 1.00 | 22 | .31 | W | 0 |
| 00 | ATOM | 3980 | | HOH | | | 4.56 | | 2.175 | | .373 | 1.00 | 24 | .90 | W | 0 |
| | ATOM | 3981 | | HOH | | | 3.92 | | 0.530 | | | 1.00 | | | W | 0 |
| | MOTA | 3982 | | HOH | | | 4.72 | | 5.239 | 102 | .749 | 1.00 | | | W | 0 |
| | | 3983 | | HOH | | | 7.79 | | 2.775 | 103 | .123 | 1.00 | | | W | 0 |
| | MOTA | | | | | | 8.31 | | 4.220 | | | 1.00 | | | W | ō |
| 55 | ATOM | 3984 | | HOH | | | | | 1.766 | | .413 | 1.00 | | | W | ŏ |
| | MOTA | 3985 | | HOH | | | 1.58 | | | | | 1.00 | 7 2 3 | 10 | W | ŏ |
| | MOTA | 3986 | | HOH | | | 4.52 | | 7.870 | | | | | | W | ŏ |
| | MOTA | 3987 | | HOH | | | 4.25 | | 8.013 | | .680 | | | | | |
| | MOTA | 3988 | | HOH | | | 5.05 | | 2.423 | | .326 | | | | W | 0 |
| 60 | MOTA | 3989 | 0 | HOH | W 40 | | 0.59 | | 3.706 | | .423 | | | | W | 0 |
| | MOTA | 3990 | 0 | HOH | W 41 | | 1.26 | | 0.306 | | .711 | | | | W | 0 |
| | ATOM | 3991 | | HOH | W 42 | | 1.11 | | 5.325 | | | | | | W | 0 |
| | ATOM | 3992 | | HOH | | 3 | 5.41 | 2 - | -7.469 | 9 83 | .691 | | | | W | 0 |
| | MOTA | 3993 | | HOH | | | 9.03 | 6 1 | .3.571 | L 83 | .635 | | | | W | 0 |
| 65 | ATOM | 3994 | | НОН | | | 3.46 | | 5.887 | 7 100 | .291 | 1.00 | 26 | .02 | W | 0 |
| | MOTA | 3995 | | НОН | | | 3.70 | | 4.144 | | | | 31 | 69 | W | 0 |
| | MOTA | 3996 | | HOH | | | 2.58 | | 4.601 | | .291 | | | | W | 0 |
| | ATOM | 3997 | | HOH | | | 2.82 | | 7.152 | | .066 | 1.00 | 30 | .03 | W | 0 |
| | MOTA | 3998 | | HOH | | | 6.65 | | 4.316 | | | | | | W | 0 |
| | ATOM | ٥٥٥٥ | , , | 11011 | ., 50 | _ | | | | | | | | | | |

| | MOTA MOTA | 3999 4000 | 0 | HOH W 51 HOH W 52 | | 25.145 115.275 -11.529 69.044 | 1.00 28.34 1.00 21.03 | W W | 0 |
|----|--------------|---------------------|---|------------------------|-------------------|----------------------------------|--------------------------|--------|---|
| | ATOM ATOM | $\frac{4001}{4002}$ | 0 | нон w 53 нон w 54 | 27.250 -6.410 | 33.402 98.412 20.233 102.747 | 1.00 26.19 1.00 32.23 | W W | 0 |
| 5 | ATOM ATOM | 4003 4004 | 0 | HOH W 55 HOH W 56 | 25.539 -3.623 | 22.652 105.834 39.874 107.173 | 1.00 40.60 1.00 43.07 | W W | 0 |
| | ATOM | 4005 | 0 | HOH W 57 | 30.894 | 4.390 71.988 | 1.00 32.39 | W | 0 |
| | ATOM ATOM | 4006 4007 | 0 | HOH W 58 HOH W 59 | 22.406 34.129 | 3.311 79.796 6.169 87.418 | 1.00 19.82 1.00 33.67 | M | 0 |
| 10 | ATOM | 4008 | 0 | HOH W 60 | -3.318 | 35.590 100.547 | 1.00 28.53 | M | 0 |
| | ATOM ATOM | 4009 4010 | 0 | HOH W 61 HOH W 62 | 23.032 -10.710 | -6.709 102.637 38.525 105.096 | 1.00 35.35 1.00 21.21 | W | 0 |
| | MOTA | 4011 | ŏ | HOH W 63 | 17.542 | 8.543 106.106 | 1.00 28.80 | W | О |
| 15 | ATOM ATOM | 4012 4013 | 0 | HOH W 64 HOH W 65 | 2.489 30.074 | 33.089 97.944 17.145 98.763 | 1.00 22.39 1.00 17.05 | W | 0 |
| 13 | ATOM | 4014 | 0 | HOH W 66 | -16.374 | 28.372 102.556 | 1.00 24.41 | M | 0 |
| | ATOM ATOM | 4015 4016 | 0 | нон W 67 нон W 68 | 9.528 23.360 | 23.065 103.276 -5.629 91.918 | 1.00 39.55 1.00 29.13 | W | 0 |
| | ATOM | 4017 | Ö | HOH W 69 | 10.550 | 28.053 110.107 | 1.00 18.71 | M | 0 |
| 20 | ATOM | 4018 | 0 | HOH W 70 HOH W 71 | -2.937 -16.268 | 25.921 114.654 35.216 117.114 | 1.00 30.39 1.00 36.27 | W | 0 |
| | ATOM ATOM | 4019 4020 | 0 | HOH W 71 HOH W 72 | 23.240 | -7.692 94.601 | 1.00 36.27 | M | ŏ |
| | MOTA | 4021 | 0 | HOH W 73 | 28.558 -15.000 | 29.902 99.941 | 1.00 37.38 | W | 0 |
| 25 | ATOM ATOM | 4022 4023 | 0 | нон W 74 нон W 75 | 5.317 | 6.861 100.111 37.793 102.522 | 1.00 27.16 1.00 30.41 | W W | 0 |
| | MOTA | 4024 | 0 | HOH W 76 | 19.168 | 23.700 110.137 | 1.00 28.91 | W | 0 |
| | MOTA MOTA | 4025 4026 | 0 | нон w 77 нон w 78 | 30.386 36.143 | -10.910 84.608 7.975 79.406 | 1.00 32.94 1.00 29.70 | W W | 0 |
| | MOTA | 4027 | О | HOH W 79 | 22.776 | 9.248 82.183 | 1.00 20.17 | W | О |
| 30 | MOTA MOTA | 4028 4029 | 0 | HOH W 81 HOH W 82 | 37.057 28.228 | -8.282 74.493 29.062 103.673 | 1.00 20.27 1.00 28.10 | W W | 0 |
| | MOTA | 4030 | 0 | HOH W 83 | -0.541 | 19.565 105.264 | 1.00 24.14 | W | 0 |
| | MOTA MOTA | $\frac{4031}{4032}$ | 0 | нон w 84 нон w 85 | 22.692 6.319 | 3.297 107.514 9.905 75.975 | 1.00 26.48 1.00 33.33 | W | 0 |
| 35 | ATOM | 4033 | ŏ | HOH W 86 | -20.077 | 32.736 123.087 | 1.00 26.22 | W | Ο |
| | MOTA | 4034 4035 | 0 | HOH W 87 HOH W 88 | 2.894 16.333 | -6.811 78.653 13.154 86.247 | 1.00 27.94 1.00 19.04 | W W | 0 |
| | ATOM ATOM | 4035 | 0 | HOH W 89 | -18.401 | 26.785 101.005 | 1.00 20.65 | W | Ö |
| 40 | MOTA | 4037 | 0 | HOH W 90 | 14.178 37.756 | 4.497 102.132 12.396 75.146 | 1.00 14.84 1.00 53.57 | W W | 0 |
| 40 | ATOM ATOM | 4038 4039 | 0 | нон w 91 нон w 92 | 5.996 | 41.146 107.575 | 1.00 31.31 | W | ŏ |
| | MOTA | 4040 | 0 | HOH W 93 | 33.958 29.435 | 9.979 93.064 24.180 93.845 | 1.00 21.64 1.00 31.70 | W W | 0 |
| | ATOM ATOM | $\frac{4041}{4042}$ | 0 | НОН W 94 НОН W 95 | -20.084 | 29.808 120.008 | 1.00 31.70 | W | Ö |
| 45 | ATOM | 4043 | 0 | HOH W 96 | 11.886 | 24.347 94.949 | 1.00 31.14 | W | 0 |
| | ATOM ATOM | $\frac{4044}{4045}$ | 0 | нон W 97 нон W 98 | 20.130 13.677 | -7.765 79.021 13.199 85.492 | 1.00 24.27 1.00 41.34 | W W | 0 |
| | ATOM | 4046 | Ō | HOH W 100 | 9.428 | 16.898 98.102 | 1.00 28.31 | W | 0 |
| 50 | ATOM ATOM | $\frac{4047}{4048}$ | 0 | нон W 101 нон W 102 | -14.681 | -12.636 81.025 35.792 88.683 | 1.00 21.44 1.00 43.48 | W W | 0 |
| | ATOM | 4049 | 0 | HOH W 103 | -7.331 | 22.775 102.908 | 1.00 21.34 | W | 0 |
| | ATOM ATOM | 4050 4051 | 0 | HOH W 104 HOH W 105 | 30.867 30.952 | -3.411 103.450 7.074 82.558 | 1.00 17.02 1.00 30.32 | W | 0 |
| | ATOM | 4052 | 0 | HOH W 106 | 0.055 | -8.254 81.647 | 1.00 44.32 | W | 0 |
| 55 | ATOM ATOM | $\frac{4053}{4054}$ | 0 | НОН W 107 НОН W 108 | 24.927 -23.807 | 13.293 82.288 32.474 120.697 | 1.00 33.73 1.00 34.73 | W | 0 |
| | ATOM | 4055 | ŏ | HOH W 109 | 9.549 | -11.066 85.205 | 1.00 32.37 | W | 0 |
| | ATOM ATOM | 4056 4057 | 0 | HOH W 110 HOH W 111 | 31.311 31.367 | -4.410 95.935 -8.798 85.899 | 1.00 36.67 1.00 24.73 | W W | 0 |
| 60 | MOTA | 4058 | ŏ | HOH W 112 | -2.685 | 32.829 97.162 | 1.00 14.26 | W | О |
| | MOTA | 4059 | 0 | HOH W 113 HOH W 114 | 31.508 14.725 | 24.004 97.423 -7.846 97.853 | 1.00 32.37 1.00 25.19 | W | 0 |
| | ATOM ATOM | 4060 4061 | 0 | HOH W 114 | -3.331 | 27.584 87.465 | 1.00 25.15 | W | ŏ |
| 05 | ATOM | 4062 | 0 | HOH W 116 | 9.759 | 12.912 73.461 | 1.00 17.17 | W | 0 |
| 65 | ATOM ATOM | 4063 4064 | 0 | HOH W 117 HOH W 118 | -9.716 20.800 | 4.459 90.108 2.961 70.582 | 1.00 32.05 1.00 30.32 | W W | 0 |
| | ATOM | 4065 | 0 | HOH W 119 | 18.183 | 35.258 107.203 | 1.00 25.90 | Ŵ | 0 |
| | ATOM ATOM | 4066 4067 | 0 | НОН W 120 НОН W 122 | 14.131 13.443 | 35.183 110.395 31.066 92.909 | 1.00 31.30 1.00 28.30 | W W | 0 |
| | | | | | | | | | |

| | ATOM | 4068 O | | нон w 123 | 5.710 25.002 114.636 1.00 50.47 W | 0 |
|----|--------------|---------------------|--------|------------------------|---|-----|
| | ATOM | 4069 0 | | HOH W 124 | -9.776 26.728 117.248 1.00 38.41 W -15.147 2.711 93.850 1.00 28.99 W | 0 |
| | MOTA | 4070 O 4071 O | | HOH W 125 HOH W 126 | 22.123 32.188 96.064 1.00 28.66 W | 0 . |
| 5 | ATOM ATOM | 4071 O 4072 O |) | HOH W 127 | 18.922 7.388 72.762 1.00 31.98 W | 0 |
| 5 | MOTA | 4073 O | | HOH W 128 | 26.078 -10.105 80.952 1.00 33.21 W 33.351 8.652 88.931 1.00 34.31 W | ŏ |
| | MOTA | 4074 O | | HOH W 129 HOH W 130 | 33.136 15.710 88.777 1.00 51.57 W | 0 |
| | MOTA MOTA | 4075 O | | HOH W 131 | 2.007 37.692 103.678 1.00 36.95 W | 0 |
| 10 | MOTA | 4077 C | | HOH W 132 HOH W 133 | 7 880 -11 049 90.515 1.00 41.06 W | ŏ |
| | ATOM ATOM | 4078 C | | HOH W 133 HOH W 134 | -11.066 28.063 82.867 1.00 45.18 W | 0 |
| | ATOM | 4080 C | | HOH W 135 | 25.936 -6.768 94.146 1.00 32.98 W | 0 |
| | MOTA | 4081 | | HOH W 136 HOH W 137 | 43.370 1.669 71.874 1.00 32.04 W 1.019 6.008 79.468 1.00 40.19 W | 0 |
| 15 | ATOM ATOM | 4082 C | _ | HOH W 137 | 34.715 13.498 101.014 1.00 53.03 W | 0 |
| | ATOM | | 5 | HOH W 139 | 22.191 11.429 81.361 1.00 41.29 W 24.467 21.102 82.091 1.00 34.83 W | 0 |
| | MOTA | | 5 | HOH W 140 HOH W 141 | 15 139 37 655 103.495 1.00 28.25 W | 0 |
| 20 | ATOM ATOM | |)) | HOH W 142 | -11.890 15.447 104.306 1.00 26.61 W | 0 |
| 20 | MOTA | | 0 | HOH W 143 | 32.110 -6.441 50.470 1.00 51 | 0 |
| | MOTA | | 0 | нон w 144 нон w 145 | 19 868 20.917 110.695 1.00 48.68 W | 0 |
| | MOTA MOTA | | 0 0 | HOH W 146 | 4.529 35.844 118.732 1.00 38.17 W | 0 |
| 25 | MOTA | 4092 | Ō | HOH W 147 | 31.420 13.080 84.897 1.00 35.77 W 5.862 33.041 95.343 1.00 42.81 W | ŏ |
| | MOTA | | 0 0 | нон W 148 нон W 149 | 36.227 -7.429 65.214 1.00 52.25 W | 0 |
| | MOTA MOTA | | 0 | HOH W 150 | 12.533 -3.257 98.974 1.00 30.04 W | 0 |
| | MOTA | | 0 | нон W 151 нон W 152 | 41.936 5.196 81.078 1.00 48.30 W 5.365 0.173 100.870 1.00 38.17 W | 0 |
| 30 | ATOM ATOM | | 0 | HOH W 152 | 18.974 10.598 76.035 1.00 27.27 W | 0 |
| | MOTA | | ŏ | HOH W 154 | -11.459 23.657 81.891 1.00 44.66 W -11.643 37.549 102.792 1.00 29.06 W | ŏ |
| | MOTA | | 0 | нон w 155 нон w 156 | 21 611 33.384 110.725 1.00 43.54 W | 0 |
| 35 | MOTA MOTA | $\frac{4101}{4102}$ | Ö | HOH W 157 | 5.082 13.359 91.364 1.00 34.56 W | 0 |
| 00 | MOTA | 4103 | 0 | HOH W 158 | -4.222 32.340 117.504 1.00 52.91 W -4.833 0.443 84.678 1.00 31.52 W | ŏ |
| | MOTA ATOM | 4104 4105 | 0 | НОН W 159 НОН W 160 | -2.712 24.390 91.588 1.00 42.37 W | 0 |
| | ATOM | 4106 | Ö | HOH W 161 | 23.968 10.013 108.083 1.00 52.17 W 39.266 7.831 70.972 1.00 30.66 W | 0 |
| 40 | MOTA | 4107 | 0 | HOH W 162 HOH W 163 | 39.266 7.831 70.972 1.00 30.66 W -6.156 19.204 110.800 1.00 49.86 W | 0 |
| | MOTA MOTA | 4108 4109 | 0 | HOH W 164 | 19.098 17.380 84.173 1.00 36.03 W | 0 |
| | MOTA | 4110 | 0 | HOH W 165 | 13.399 33.954 93.836 1.00 36.17 W -31.448 25.540 114.441 1.00 37.50 W | ŏ |
| 45 | MOTA | $\frac{4111}{4112}$ | 0 | нон W 166 нон W 167 | 13.302 14.583 106.224 1.00 21.88 W | 0 |
| 45 | MOTA MOTA | 4113 | ŏ | HOH W 169 | 1.752 26.748 97.241 1.00 37.67 W 27.718 0.693 62.087 1.00 46.32 W | 0 |
| | ATOM | 4114 | 0 | нон w 170 нон w 171 | 28 912 -5.883 98.061 1.00 45.53 W | Ō |
| | ATOM ATOM | 4115 4116 | 0 | HOH W 171 HOH W 172 | 12.144 -6.132 99.269 1.00 28.03 W | 0 |
| 50 | ATOM | 4117 | 0 | HOH W 173 | 9.713 14.070 99.156 1.00 36.36 W 44.241 3.007 80.980 1.00 55.52 W | ŏ |
| | MOTA | 4118 | 0 | нон w 174 нон w 175 | -2.145 9.708 89.227 1.00 30.25 W | 0 |
| | MOTA MOTA | 4119 4120 | 0 | HOH W 176 | 21.259 13.911 103.297 1.00 46.50 W | 0 |
| | MOTA | 4121 | 0 | HOH W 177 | 28.628 2.356 108.048 1.00 35.93 W -3.113 20.410 91.180 1.00 49.91 W | 0 |
| 55 | ATOM ATOM | 4122 4123 | 0 | нон w 178 нон w 179 | 9.943 40.130 105.661 1.00 49.34 W | 0 |
| | ATOM | 4124 | ŏ | HOH W 180 | -14.721 37.561 104.779 1.00 37.09 W 0.350 -13.390 93.145 1.00 42.85 W | 0 |
| | ATOM | | 0 | нон W 181 нон W 182 | -16 751 30.840 125.808 1.00 43.38 W | 0 |
| 60 | MOTA MOTA | 4400 | 0 | HOH W 182 | 5.022 10.944 94.912 1.00 36.63 W | 0 |
| 00 | MOTA | 4128 | 0 | HOH W 184 | 4/.344 -3.1/2 03.012 1.00 44 43 | ŏ |
| | ATOM | | 0 | НОН W 185 НОН W 186 | 11 422 0.781 69.608 1.00 50.67 W | 0 |
| | ATOM ATOM | | 0 | HOH W 187 | 1.340 12.706 88.912 1.00 17.04 W | 0 |
| 65 | ATOM | 4132 | 0 | HOH W 188 | 9 004 12 970 81.421 1.00 51.36 W | 0 |
| | ATOM ATOM | | 0 | нон W 189 нон W 191 | 30.121 9.526 83.001 1.00 30.35 W | 0 |
| | ATOM | | 0 | нон w 192 | -13.167 21.122 108.317 1.00 36.08 W -17.245 22.145 114.082 1.00 45.19 W | 0 |
| | ATOM | 4136 | 0 | нон W 193 | 2,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,,, | |
| | | | | | 173 | |

| | ATOM | 4137 | 0 | нон w 194 | | 0 35.80 | M | 0 |
|----|--------------|----------------|---|------------------------|---|----------------------|------------------|-----|
| | MOTA | 4138 | 0 | HOH W 195 | 25.255 | 0 33.67 0 35.43 | W | 0 |
| | ATOM | 4139 | 0 | HOH W 196 | 1.000 | 0 26.66 | W | Ö |
| _ | ATOM | 4140 | 0 | нон w 197 нон w 198 | | 0 43.04 | M | ŏ |
| 5 | ATOM ATOM | $4141 \\ 4142$ | 0 | HOH W 199 | 8.986 -7.658 77.984 1.0 | 0 41.83 | W | 0 |
| | ATOM | 4143 | 0 | HOH W 200 | -18.535 14.030 99.271 1.0 | 0 42.15 | M | 0 |
| | ATOM | 4144 | ŏ | HOH W 201 | 35.091 -0.808 99.802 1.0 | | M | 0 |
| | ATOM | 4145 | 0 | HOH W 203 | 2.101 | 0 74.49 | M | 0 |
| 10 | MOTA | 4146 | 0 | HOH W 204 | | 0 34.52 | M | 0 |
| | MOTA | 4147 | 0 | HOH W 205 | 10.210 10.030 1000 | 0 37.42 0 42.78 | W | 0 |
| | MOTA | 4148 | 0 | нон w 206 | | 00 42.78 | W | ŏ |
| | ATOM | 4149 | 0 | нон W 207 нон W 208 | | 0 50.13 | M | ŏ |
| 45 | MOTA | 4150 4151 | 0 | HOH W 208 | | 0 33.69 | W | 0 |
| 15 | MOTA MOTA | 4152 | Ö | HOH W 212 | | 0 37.61 | W | 0 |
| | ATOM | 4153 | ŏ | HOH W 214 | | 0 30.67 | W | 0 |
| | MOTA | 4154 | ŏ | HOH W 215 | | 0 30.32 | W | 0 |
| | ATOM | 4155 | 0 | HOH W 216 | | 00 39.11 | M | 0 |
| 20 | MOTA | 4156 | 0 | TIOIT W | | 00 31.57 | W | 0 |
| | MOTA | 4157 | 0 | HOH W 218 | | 00 46.35 00 51.22 | W W | Ö |
| | ATOM | 4158 | 0 | HOH W 219 | | 00 63.55 | W | ŏ |
| | ATOM | 4159 4160 | 0 | HOH W 220 HOH W 221 | | 00 39.00 | W | Ö |
| 25 | ATOM ATOM | 4161 | 0 | HOH W 221 | | 00 62.58 | W | 0 |
| 20 | ATOM | 4162 | ŏ | HOH W 223 | 16.250 35.597 101.623 1.0 | 00 29.57 | W | 0 |
| | ATOM | 4163 | Ō | HOH W 224 | 20.5.2 | 00 41.21 | W | 0 |
| | ATOM | 4164 | 0 | HOH W 225 | | 00 39.22 | W | 0 |
| | MOTA | 4165 | 0 | нон w 226 | 10.200 | 00 52.06 00 28.91 | W | 0 |
| 30 | MOTA | 4166 | 0 | HOH W 227 | =:00: | | W | Ö |
| | ATOM | 4167 | 0 | HOH W 228 HOH W 229 | 20.700 22.012 | 00 44.90 | W | ŏ |
| | ATOM ATOM | 4168 4169 | 0 | HOH W 239 | | 00 47.35 | W | 0 |
| | ATOM | 4170 | Ö | HOH W 231 | | 00 37.92 | \mathbf{W}^{c} | 0 |
| 35 | MOTA | 4171 | ŏ | HOH W 232 | 26.302 27.216 105.852 1.0 | | M | 0 |
| 00 | MOTA | 4172 | ō | HOH W 233 | | 00 35.69 | M | . 0 |
| | ATOM | 4173 | 0 | HOH W 234 | | 00 56.46 | W | 0 |
| | MOTA | 4174 | 0 | нон w 235 | | 00 56.82 00 46.16 | W W | 0 |
| | MOTA | 4175 | 0 | нон w 236 | | 00 40.10 | W | Ö |
| 40 | MOTA | 4176 | 0 | нон w 237 нон w 238 | | 00 32.27 | M | ŏ |
| | MOTA MOTA | 4177 4178 | 0 | HOH W 239 | | 00 66.22 | M | 0 |
| | ATOM | 4179 | Ö | HOH W 240 | | 00 38.96 | W | 0 |
| | ATOM | 4180 | ŏ | HOH W 242 | -4.347 7.089 83.943 1. | 00 34.28 | M | 0 |
| 45 | ATOM | 4181 | 0 | HOH W 244 | 20,000 | 00 35.74 | M | 0 |
| | MOTA | 4182 | 0 | HOH W 245 | | 00 98.33 | W | 0 |
| | MOTA | 4183 | 0 | HOH W 246 | | 00 60.71 00 37.52 | M | 0 |
| | ATOM | 4184 | 0 | HOH W 247 | | 00 37.52 | W | ŏ |
| F0 | MOTA | 4185 | 0 | нон w 248 нон w 249 | | 00 42.13 | W | Ō |
| 50 | ATOM ATOM | 4186 4187 | 0 | HOH W 250 | | 00 34.13 | W | 0 |
| | ATOM | 4188 | ŏ | HOH W 251 | 12.546 26.526 89.169 1. | 00 75.55 | W | 0 |
| | ATOM | 4189 | ō | HOH W 252 | 15.820 -5.443 71.698 1. | 00 64.76 | W | 0 |
| | ATOM | 4190 | 0 | HOH W 253 | | 00 45.55 | W | 0 |
| 55 | MOTA | 4191 | 0 | HOH W 254 | | 00 39.90 00 43.29 | W W | 0 |
| | MOTA | 4192 | 0 | HOH W 255 | • | 00 50.06 | W | ŏ |
| | ATOM | 4193 | 0 | HOH W 256 | | 00 42.11 | W | ŏ |
| | MOTA | 4194 4195 | 0 | HOH W 257 HOH W 258 | | 00 48.63 | W | Ō |
| 60 | ATOM ATOM | 4196 | 0 | HOH W 259 | 26.271 16.951 106.835 1. | 00 28.76 | W | 0 |
| 00 | MOTA | 4197 | ŏ | HOH W 260 | 21.231 10.692 77.782 1. | 00 52.78 | W | 0 |
| | ATOM | 4198 | ŏ | HOH W 261 | 8.597 31.178 114.621 1. | 00 29.98 | \mathbf{W} | 0 |
| | MOTA | 4199 | 0 | HOH W 263 | | 00 49.49 | W | 0 |
| | MOTA | 4200 | 0 | HOH W 264 | | 00 43.50 | W W | 0 |
| 65 | ATOM | 4201 | 0 | нон w 265 | | 00 40.59 | W | 0 |
| | MOTA | 4202 | 0 | HOH W 266 | 33.611 10.760 95.480 1. -13.163 9.376 82.701 1. | 00 91.44 | W | ŏ |
| | MOTA | 4203 | 0 | нон W 268 нон W 269 | -13.163 9.376 82.761 1. -10.588 -3.736 92.548 1. | 00 48.91 | W | ŏ |
| | MOTA MOTA | 4204 4205 | 0 | HOH W 200 | | 00 46.59 | W | 0 |
| | 121011 | | - | | | | | |

| | | | | | | 22 246 22 225 | 1 00 70 00 | 7.7 | _ |
|----------|--------------|--------------|---|------------------------|--------------------|----------------------------------|--------------------------|-----|---|
| | ATOM | 4206 | 0 | HOH W 271 | -15.610 | 30.916 83.905 | 1.00 72.20 1.00 40.04 | W | 0 |
| | MOTA | 4207 | 0 | HOH W 272 | 8.482 | -2.678 100.994 39.625 106.340 | 1.00 40.04 | W | Ö |
| | MOTA | 4208 | 0 | нон w 273 нон w 274 | -14.819 -15.862 | 27.341 124.046 | 1.00 32.00 | W | ŏ |
| = | MOTA MOTA | 4209 4210 | 0 | HOH W 274 | 0.355 | 7.737 78.018 | 1.00 39.51 | W | ŏ |
| 5 | ATOM | 4211 | ŏ | HOH W 275 | 11.649 | 6.543 73.332 | 1.00 62.29 | W | Ō |
| | ATOM | 4212 | Ö | HOH W 277 | 13.896 | 1.911 70.069 | 1.00 36.22 | W | 0 |
| | ATOM | 4213 | ŏ | HOH W 279 | 11.226 | 9.285 70.225 | 1.00 37.33 | W | 0 |
| | ATOM | 4214 | ŏ | HOH W 280 | 17.596 | 11.506 73.709 | 1.00 37.13 | W | 0 |
| 10 | ATOM | 4215 | ō | HOH W 281 | 22.601 | 8.046 77.458 | 1.00 84.20 | M | 0 |
| • - | ATOM | 4216 | 0 | HOH W 282 | 22.007 | 2.832 75.959 | 1.00 60.94 | W | 0 |
| | MOTA | 4217 | 0 | HOH W 283 | 14.332 | 0.684 101.417 | 1.00 26.51 | W | 0 |
| | MOTA | 4218 | 0 | HOH W 284 | 17.488 | 14.803 74.520 | 1.00 50.25 | W | 0 |
| | MOTA | 4219 | 0 | HOH W 285 | 11.672 | 12.725 82.121 | 1.00 31.27 1.00 49.99 | M | 0 |
| 15 | ATOM | 4220 | 0 | HOH W 286 | 13.338 | 15.638 79.654 15.666 77.915 | 1.00 49.99 | W | Ö |
| | ATOM | 4221 | 0 | HOH W 287 HOH W 288 | 15.476 -19.019 | 18.128 91.748 | 1.00 57.76 | W | ő |
| | MOTA | 4222 | 0 | HOH W 289 | -19.019 | 20.525 92.776 | 1.00 57.70 | W | ŏ |
| | MOTA MOTA | 4223 4224 | 0 | HOH W 290 | -21.754 | 17.779 92.013 | 1.00 70.60 | M | Ö |
| 20 | ATOM | 4225 | ŏ | HOH W 291 | -7.681 | 20.732 86.926 | 1.00 30.75 | W | 0 |
| 20 | MOTA | 4226 | ŏ | HOH W 292 | -18.672 | 16.770 99.341 | 1.00 72.88 | M | 0 |
| | ATOM | 4227 | ŏ | HOH W 293 | 41.053 | -10.007 75.389 | 1.00 40.19 | W | 0 |
| | ATOM | 4228 | 0 | HOH W 294 | 15.967 | 34.561 95.189 | 1.00 32.39 | M | 0 |
| | ATOM | 4229 | 0 | нон w 295 | 3.242 | 22.750 99.080 | 1.00 42.03 | M | 0 |
| 25 | MOTA | 4230 | 0 | нон w 296 | 42.034 | 1.021 85.260 | 1.00 31.00 | W | 0 |
| | MOTA | 4231 | 0 | HOH W 297 | 34.100 | -8.318 85.997 | 1.00 20.43 1.00 51.52 | W | 0 |
| | ATOM | 4232 | 0 | HOH W 298 | 26.478 34.395 | 33.532 95.995 6.694 89.928 | 1.00 51.52 1.00 53.02 | W | 0 |
| | MOTA | 4233 | 0 | нон w 299 нон w 300 | -0.985 | 37.065 99.982 | 1.00 39.51 | W | ŏ |
| 20 | ATOM ATOM | 4234 4235 | 0 | HOH W 300 | -0.252 | 34.259 98.319 | 1.00 40.18 | W | ō |
| 30 | MOTA | 4236 | Ö | HOH W 302 | 1.043 | 37.976 101.110 | 1.00 50.67 | W | 0 |
| | ATOM | 4237 | ŏ | HOH W 303 | 13.169 | 27.347 107.852 | 1.00 .46.98 | W | 0 |
| | MOTA | 4238 | ŏ | HOH W 304 | 2.617 | -8.808 82.550 | 1.00 34.55 | W | 0 |
| | ATOM | 4239 | O | HOH W 306 | -24.119 | 34.693 121.849 | 1.00 38.49 | W | 0 |
| 35 | ATOM | 4240 | 0 | HOH W 307 | -21.110 | 33.926 125.264 | 1.00 35.91 | W | 0 |
| | ATOM | 4241 | 0 | HOH W 308 | -22.717 | 35.450 124.405 | 1.00 40.22 | M | 0 |
| | ATOM | 4242 | 0 | нон w 309 | 14.431 | -7.080 100.358 | 1.00 40.89 | W | 0 |
| | ATOM | 4243 | 0 | HOH W 310 | -1.633 | 26.170 89.620 23.415 92.259 | 1.00 32.95 1.00 48.52 | W | 0 |
| | ATOM | 4244 | 0 | HOH W 311 | -0.715 15.583 | 23.415 92.259 37.247 111.051 | 1.00102.38 | M | ő |
| 40 | MOTA | 4245 | 0 | нон W 312 нон W 313 | 49.127 | -4.716 84.592 | 1.00102.30 | M | ŏ |
| | ATOM ATOM | 4246 4247 | 0 | HOH W 315 | 4.543 | 25.776 97.442 | 1.00 20.30 | W | ō |
| | ATOM | 4248 | Ö | HOH W 317 | 13.219 | -2.231 96.766 | 1.00 26.75 | W | 0 |
| | MOTA | 4249 | ŏ | HOH W 318 | -1.027 | 12.136 89.956 | 1.00 30.29 | M | 0 |
| 45 | ATOM | 4250 | 0 | HOH W 319 | 24.455 | -0.869 84.238 | 1.00 47.96 | M | 0 |
| | MOTA | 4251 | 0 | HOH W 321 | 7.387 | 26.214 95.885 | 1.00 43.12 | M | 0 |
| | MOTA | 4252 | 0 | нон w 323 | -10.121 | 37.815 100.499 | 1.00 26.17 | M | 0 |
| | MOTA | 4253 | 0 | HOH W 324 | 44.204 | -8.495 89.166 | 1.00 41.06 1.00 24.87 | W | 0 |
| | ATOM | 4254 | 0 | HOH W 325 | 16.219 16.724 | 0.595 103.250 6.735 108.041 | 1.00 24.87 | W | ŏ |
| 50 | ATOM | 4255 4256 | 0 | нон w 326 нон w 327 | -5.658 | 41.985 114.043 | 1.00 41.88 | W | Ö |
| | ATOM ATOM | 4257 | 0 | HOH W 327 | 30.517 | 7.926 72.820 | 1.00 24.86 | W | Ō |
| | ATOM | 4258 | ŏ | HOH W 329 | -4.229 | 13.443 105.886 | 1.00 42.46 | W | 0 |
| | MOTA | 4259 | ŏ | HOH W 330 | 9.856 | -2.127 98.647 | 1.00 29.78 | W | 0 |
| 55 | MOTA | 4260 | ō | HOH W 331 | 32.200 | 13.062 101.692 | 1.00 46.72 | W | 0 |
| | ATOM | 4261 | 0 | HOH W 332 | 11.618 | 16.977 87.587 | 1.00 38.22 | M | 0 |
| | MOTA | 4262 | 0 | HOH W 334 | 13.863 | 35.533 100.193 | 1.00 38.69 | W | 0 |
| | MOTA | 4263 | 0 | HOH W 335 | 3.202 | 20.353 103.614 | 1.00 41.76 | W | 0 |
| | ATOM | 4264 | 0 | HOH W 336 | -0.265 | 25.481 112.882 | 1.00 45.85 1.00 40.43 | W | o |
| 60 | ATOM | 4265 | 0 | HOH W 337 | 33.088 -10.753 | 17.503 92.709 19.811 115.192 | 1.00 40.43 | W | ŏ |
| | MOTA | 4266 | 0 | нон w 338 нон w 339 | 5.702 | 24.463 117.434 | 1.00 32.03 | W | ŏ |
| | ATOM | 4267 4268 | 0 | HOH W 339 | 36.083 | 5.104 86.455 | 1.00 32.03 | W | ŏ |
| | MOTA MOTA | 4268 | 0 | HOH W 340 | 45.308 | | 1.00 43.84 | W | ŏ |
| 65 | ATOM | 4270 | ŏ | HOH W 342 | -3.013 | 2.927 80.584 | 1.00 48.18 | W | 0 |
| 00 | ATOM | 4271 | ŏ | HOH W 343 | -8.584 | 2.810 102.723 | 1.00 45.47 | W | 0 |
| | ATOM | 4272 | O | HOH W 344 | 14.270 | 31.214 111.267 | 1.00 53.23 | M | 0 |
| | MOTA | 4273 | 0 | HOH W 345 | 5.303 | 5.466 73.316 | 1.00 35.97 | W | 0 |
| | ATOM | 4274 | 0 | нон w 346 | 5.884 | 14.859 94.569 | 1.00 34.36 | W | 0 |
| | | | | | | | | | |

| | ATOM | 4275 | 0 | НОН W 347 НОН W 348 | 13.766 -10.804 94.639 1.00 37.55 28.817 -6.638 95.408 1.00 46.05 | W | 0 |
|----|--------------|---------------|---|------------------------|--|--------|---|
| | ATOM ATOM | 4276 4277 | 0 | HOH W 349 | -16.201 4.012 101.225 1.00 55.36 | W | 0 |
| 5 | ATOM ATOM | ·4278 4279 | 0 | нон W 350 нон W 351 | -11.930 40.337 106.636 1.00 34.71 | M | 0 |
| | ATOM | 4280 4281 | 0 | нон w 352 нон w 353 | 14.848 22.833 108.104 1.00 32.58 4.331 11.520 83.240 1.00 65.30 | W | 0 |
| | ATOM ATOM | 4282 | Ö | HOH W 354 | -30.188 27.123 112.476 1.00 54.95 | W | 0 |
| 10 | ATOM ATOM | 4283 4284 | 0 | нон w 355 нон w 356 | 0.831 37.120 115.463 1.00 45.14 39.804 -9.143 67.597 1.00 38.07 | W | 0 |
| 10 | MOTA | 4285 | 0 | HOH W 357 | -5.193 41.092 118.296 1.00 49.38 | W W | 0 |
| | MOTA MOTA | 4286 4287 | 0 | нон w 358 нон w 359 | 2.404 30.953 94.996 1.00 43.81 | W | 0 |
| | ATOM | 4288 | 0 | HOH W 360 | 5.633 -10.209 96.938 1.00 33.82 4.540 -6.167 100.513 1.00 39.66 | W | 0 |
| 15 | ATOM ATOM | 4289 4290 | 0 | НОН W 361 НОН W 362 | -19.660 12.268 100.884 1.00 27.40 | W | 0 |
| | ATOM | 4291 | 0 | нон w 363 | 46.225 -3.464 88.101 1.00 43.37 | W W | 0 |
| | ATOM ATOM | 4292 4293 | 0 | нон w 364 нон w 365 | 17.099 11.410 108.574 1.00 47.12 | W | 0 |
| 20 | MOTA | 4294 | 0 | HOH W 366 | 26.600 2.351 110.176 1.00 37.38 -22.520 39.595 116.261 1.00 49.47 | W W | 0 |
| | ATOM ATOM | 4295 4296 | 0 | нон W 367 нон W 368 | 0.313 25.144 94.624 1.00 40.92 | W | 0 |
| | MOTA | 4297 | 0 | нон w 369 нон w 370 | 20.613 -10.182 77.986 1.00 37.72 22.771 6.260 79.455 1.00 47.23 | W | 0 |
| 25 | MOTA ATOM | 4298 4299 | 0 | HOH W 371 | 14.209 -9.494 101.679 1.00 50.86 | W | 0 |
| | ATOM | 4300 4301 | 0 | нон w 372 нон w 373 | 32.180 -13.182 64.680 1.00 31.90 -15.578 22.302 119.158 1.00 67.22 | W | 0 |
| | MOTA MOTA | 4302 | ŏ | HOH ₩ 374 | -5.806 33.729 119.651 1.00 78.83 | W | 0 |
| 30 | MOTA MOTA | 4303 4304 | 0 | нон w 375 нон w 376 | 5.261 41.524 122.294 1.00 64.79 -26.827 27.798 95.626 1.00 52.39 | W | 0 |
| 30 | MOTA | 4305 | 0 | HOH W 377 | -0.392 20.708 96.954 1.00 47.09 | W | 0 |
| | ATOM ATOM | 4306 4307 | 0 | нон w 378 нон w 379 | 38.359 3.116 87.840 1.00 51.46 -8.697 -6.590 90.186 1.00 37.82 | M | ŏ |
| | ATOM | 4308 | 0 | HOH W 380 | 34.329 -8.438 63.764 1.00 43.15 25.046 4.206 109.068 1.00 36.85 | W | 0 |
| 35 | ATOM ATOM | 4309 4310 | 0 | нон W 381 нон W 382 | -12.307 4.812 90.954 1.00 54.83 | W | 0 |
| | MOTA | 4311 | 0 | HOH W 383 | 22.346 0.999 109.244 1.00 55.83 20.145 33.493 94.808 1.00 33.85 | W W | 0 |
| | ATOM ATOM | 4312 4313 | 0 | нон W 384 нон W 385 | 17.103 17.604 111.486 1.00 58.32 | W | 0 |
| 40 | ATOM | 4314 | 0 | нон w 386 нон w 387 | -19.799 34.573 91.860 1.00 30.28 14.665 36.499 114.334 1.00 75.56 | W | 0 |
| | ATOM ATOM | 4315 4316 | 0 | HOH W 388 | 7.042 35.670 94.968 1.00 48.07 | M | 0 |
| | MOTA | 4317 4318 | 0 | нон w 389 нон w 390 | 32.245 -16.178 70.702 1.00 49.01 10.283 21.058 100.027 1.00 84.17 | W | 0 |
| 45 | ATOM ATOM | 4319 | 0 | HOH W 391 | 34.895 7.447 103.148 1.00 40.35 | W | 0 |
| | MOTA MOTA | 4320 4321 | 0 | нон W 392 нон W 393 | -25.110 16.204 100.371 1.00 50.31 -25.389 34.708 117.495 1.00 48.66 | W | 0 |
| | ATOM | 4322 | ŏ | HOH W 394 | 11.890 21.970 101.820 1.00 68.28 | W | 0 |
| 50 | MOTA MOTA | 4323 4324 | 0 | нон w 395 нон w 396 | 45.837 -5.824 89.349 1.00 28.55 -8.379 40.188 104.608 1.00 50.71 | W | 0 |
| 00 | MOTA | 4325 | 0 | нон w 397 | -2.215 0.600 81.682 1.00 55.91 | W | 0 |
| | MOTA MOTA | 4326 4327 | 0 | нон w 398 нон w 399 | 24.028 8.821 110.407 1.00 40.67 | W | 0 |
| | MOTA | 4328 | 0 | HOH W 400 | 4.868 30.432 91.498 1.00 63.30 -13.446 0.549 94.109 1.00 38.55 | W W | 0 |
| 55 | ATOM ATOM | 4329 4330 | 0 | нон w 401 нон w 402 | -14.032 30.272 124.462 1.00 67.33 | W | 0 |
| | MOTA | 4331 | 0 | HOH W 403 | -8.252 25.376 115.719 1.00 72.04 -19.618 7.134 97.108 1.00 69.74 | W | 0 |
| | ATOM ATOM | 4332 4333 | 0 | нон W 404 нон W 405 | 43.024 -2.573 87.596 1.00 47.06 | W | 0 |
| 60 | MOTA | 4334 | 0 | нон W 406 нон W 407 | -8.280 39.609 100.109 1.00 45.22 13.386 -2.161 101.138 1.00 40.32 | W | 0 |
| | ATOM ATOM | 4335 4336 | 0 | HOH W 408 | 1.781 -3.496 73.915 1.00 35.10 | W | 0 |
| | MOTA | 4337 | 0 | нон W 409 нон W 410 | -19.493 33.560 127.412 1.00 52.12 -12.357 32.930 84.450 1.00 55.63 | W W | 0 |
| 65 | MOTA MOTA | 4338 4339 | 0 | HOH W 411 | -16.396 41.453 106.252 1.00 67.78 | M | 0 |
| | ATOM | 4340 4341 | 0 | HOH W 412 HOH W 413 | 9.259 22.383 107.628 1.00 62.67 26.452 10.638 108.233 1.00 55.75 | W | 0 |
| | MOTA MOTA | 4342 | 0 | HOH W 414 | 3.629 26.004 108.637 1.00 32.70 | W | 0 |
| | ATOM | 4343 | 0 | HOH W 415 | 15.226 13.844 73.002 1.00 48.60 | M | 0 |

| | ATOM ATOM ATOM | 4344 O 4345 O 4346 O | HOH W 416 HOH W 417 HOH W 418 | 1.142 27.132 93.054 1.00 41.48 -8.715 22.235 116.597 1.00 46.49 14.671 -10.428 90.692 1.00 44.76 | W O W O W O W O |
|----|--------------------------------------|--|---|--|---------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM | 4347 O 4348 O 4349 O 4350 O 4351 O | HOH W 419 HOH W 420 HOH W 421 HOH W 422 HOH W 423 | 8.057 17.800 101.961 1.00 51.89 29.708 7.490 70.081 1.00 36.19 18.102 4.689 108.132 1.00 65.88 20.158 13.014 111.569 1.00 56.69 | W O W O W O |
| 10 | ATOM ATOM ATOM ATOM | 4352 O 4353 O 4354 O 4355 O | HOH W 424 HOH W 425 HOH W 426 HOH W 427 | 24.783 24.390 107.699 1.00 68.92 33.410 -5.505 95.203 1.00 42.38 35.004 -3.766 95.192 1.00 35.89 | W O W O W O |
| 15 | MOTA MOTA MOTA MOTA MOTA MOTA | 4356 O 4357 O 4358 O 4359 O 4360 O | HOH W 428 HOH W 429 HOH W 430 HOH W 431 HOH W 432 | 31.902 10.936 83.768 1.00 50.77 20.413 14.829 81.652 1.00 86.25 32.924 22.614 95.004 1.00 57.23 17.143 27.068 92.217 1.00 41.94 | W O W O W O |
| 20 | MOTA MOTA ATOM MOTA | 4361 O 4362 O 4363 O 4364 O | HOH W 433 HOH W 434 HOH W 435 HOH W 436 HOH W 437 | 17.696 29.224 90.849 1.00 44.20 6.235 13.909 97.039 1.00 36.25 15.368 1.745 105.621 1.00 65.45 12.352 2.448 102.309 1.00 56.90 17.216 -1.654 103.171 1.00 64.25 | W O W O W O W O |
| 25 | ATOM ATOM ATOM ATOM ATOM | 4365 O 4366 O 4367 O 4368 O 4369 O | HOH W 438 HOH W 439 HOH W 440 HOH W 441 | -24.467 21.964 97.052 1.00 59.17 6.899 37.197 100.238 1.00 53.34 -5.836 25.471 114.752 1.00 49.14 -17.656 23.630 116.338 1.00 60.48 | W O W O W O W O W O |
| 30 | MOTA MOTA MOTA MOTA MOTA | 4370 O 4371 O 4372 O 4373 O 4374 O | HOH W 444 HOH W 445 | 39.860 6.346 67.021 1.00 32.01 42.143 8.359 69.500 1.00 39.71 -8.339 -3.324 88.589 1.00 48.59 -5.439 -2.506 84.631 1.00 49.07 | W O W O |
| 35 | ATOM MOTA MOTA MOTA | 4375 O 4376 O 4377 O 4378 O | HOH W 447 HOH W 448 HOH W 449 HOH W 450 | 10.114 9.300 105.299 1.00 55.06 16.239 -12.467 79.695 1.00 48.81 12.931 14.962 82.732 1.00 55.97 15.033 16.025 83.698 1.00 55.49 10.617 15.905 83.861 1.00 54.71 | W O W O W O W O |
| | ATOM ATOM ATOM ATOM | 4379 C 4380 C 4381 C 4382 C | HOH W 452 HOH W 454 HOH W 455 | 10.617 15.905 83.861 1.00 54.71 -5.587 14.189 96.637 1.00 17.19 -2.694 14.148 88.813 1.00 39.38 3.241 25.419 113.472 1.00 35.59 6.666 28.248 94.111 1.00 31.20 | W O W O W O |
| 40 | ATOM ATOM ATOM ATOM | 4383 C 4384 C 4385 C 4386 C | HOH W 457 HOH W 458 HOH W 459 | 4.912 26.581 118.595 1.00 33.12 13.177 32.164 114.127 1.00 57.36 25.786 35.921 98.725 1.00 58.99 22.635 4.638 74.051 1.00 46.06 | W O W O W O |
| 45 | ATOM ATOM ATOM ATOM | | HOH W 461 HOH W 462 HOH W 463 | 17.322 37.394 105.719 1.00 31.09 -7.224 20.703 114.851 1.00 39.30 35.611 11.671 98.382 1.00 46.52 29.883 -13.953 62.902 1.00 57.02 | W O W O W O |
| 50 | ATOM ATOM ATOM ATOM ATOM | 4392 (4393 (4394 (| HOH W 464 HOH W 465 HOH W 466 HOH W 467 HOH W 468 | 31.809 -8.822 91.814 1.00 48.95 -4.260 7.670 89.713 1.00 47.18 10.396 24.915 91.432 1.00 40.35 25.263 11.071 82.716 1.00 54.15 | M O M O |
| 55 | MOTA MOTA MOTA | 4396 4397 4398 4399 | O HOH W 469 O HOH W 470 O HOH W 471 O HOH W 472 | 38.248 5.442 99.845 1.00 42.81 36.347 9.341 100.618 1.00 34.65 -16.914 41.482 111.141 1.00 42.00 -9.184 24.264 81.849 1.00 47.30 40.726 1.808 66.833 1.00 43.72 | W O W O W O W O |
| 60 | ATOM ATOM ATOM ATOM | 4401 4402 4403 | O HOH W 473 O HOH W 474 O HOH W 475 O HOH W 476 O HOH W 477 | 31.808 -18.642 70.728 1.00 37.59 16.188 22.858 110.296 1.00 49.77 3.509 2.536 103.295 1.00 42.84 11 289 41.122 108.943 1.00 45.98 | W O W O W O |
| 65 | MOTA MOTA MOTA MOTA MOTA | 4405 4406 4407 | O HOH W 478 O HOH W 479 O HOH W 480 O HOH W 481 | 36.903 -5.044 64.038 1.00 55.21 -6.947 8.034 91.049 1.00 52.73 29.751 -15.588 72.186 1.00 39.77 -19.537 40.486 107.195 1.00 44.19 | M O M O |
| 03 | ATOM MOTA MOTA MOTA | 4409 4410 4411 | O HOH W 482 O HOH W 483 O HOH W 484 O HOH W 485 | 13.213 -5.095 67.720 1.00 60.90 49.568 -7.870 76.168 1.00 56.88 20.138 10.494 110.659 1.00 51.35 23.477 20.576 109.910 1.00 40.59 | W O W O W O |
| | | | | 177 | |

| | A.T.OM | 4413 | U | HOH W 486 | 17.274 | 23.443 | 92.256 | 1.00 20.56 | W | _ |
|----|--------|------|-----|-----------|----------|---------|------------|------------|--------|---|
| | ATOM | 4414 | 0 | HOH W 487 | -3.839 | 23.924 | 116.158 | 1.00 53.03 | W | 0 |
| | ATOM | 4415 | 0 | HOH W 488 | -9.415 | 30.760 | 123.636 | 1.00 52.62 | W | - |
| | MOTA | 4416 | 0 | HOH W 489 | -1.387 | 9.782 | 78.997 | 1.00 53.83 | | 0 |
| 5 | ATOM | 4417 | . 0 | HOH W 490 | 9.922 | -7.536 | 74.819 | 1.00 56.15 | W | 0 |
| | ATOM | 4418 | 0 | HOH W 491 | -19.282 | 13.510 | 103.374 | 1.00 42.49 | W | 0 |
| | ATOM | 4419 | 0 | HOH W 492 | 5.004 | 29.828 | 93.747 | 1.00 45.34 | | 0 |
| | MOTA | 4420 | 0 | HOH W 493 | 17.415 | -8.223 | 91.913 | 1.00 43.34 | W | 0 |
| | ATOM | 4421 | 0 | HOH W 494 | -12.983 | 20.330 | 105.539 | 1.00 54.57 | W | 0 |
| 10 | ATOM | 4422 | 0 | HOH W 495 | -7.159 | 22.883 | 83.768 | 1.00 46.62 | W | 0 |
| | ATOM | 4423 | 0 | HOH W 496 | 37.991 | -8.468 | 95.150 | 1.00 40.02 | W W | 0 |
| | MOTA | 4424 | 0 | HOH W 497 | 6.698 | 22.515 | 106.540 | 1.00 30.24 | W | 0 |
| | ATOM | 4425 | 0 | HOH W 498 | 0.537 | 27.673 | 90.158 | 1.00 31.07 | W | 0 |
| | ATOM | 4426 | 0 | HOH W 499 | • | -10.554 | 82.991 | 1.00 43.73 | W | 0 |
| 15 | ATOM | 4427 | 0 | HOH W 500 | -9.156 | 36.949 | 84.009 | 1.00 72.95 | W | 0 |
| | ATOM | 4428 | 0 | HOH W 501 | -33.297 | 21.816 | 110.516 | 1.00 49.38 | W | 0 |
| | ATOM | 4429 | 0 | HOH W 502 | | -12.296 | 83.500 | 1.00 49.38 | W | 0 |
| | ATOM | 4430 | 0 | HOH W 503 | -0.797 | 13.710 | 92.437 | 1.00 67.43 | | 0 |
| | ATOM | 4431 | 0 | HOH W 504 | -4.021 | -6.785 | 82.556 | 1.00 66.42 | W W | 0 |
| 20 | ATOM | 4432 | 0 | HOH W 505 | 39.144 | -0.596 | 89.054 | 1.00 60.42 | W | 0 |
| | ATOM | 4433 | 0 | HOH W 506 | -4.755 | -6.160 | 85.441 | 1.00 49.25 | M | 0 |
| | ATOM | 4434 | 0 | HOH W 507 | 28.668 - | -12.917 | 86.013 | 1.00 72.20 | W | 0 |
| | ATOM | 4435 | 0 | HOH W 508 | | 13.358 | 85.255 | 1.00 72.20 | W | 0 |
| | MOTA | 4436 | 0 | HOH W 509 | 1.611 | | 103.500 | 1.00 63.21 | W | 0 |
| 25 | MOTA | 4437 | 0 | HOH W 510 | -16.935 | 38.862 | 97.751 | 1.00 33.21 | | 0 |
| | TER | 4438 | | HOH W 510 | | | - , . , 51 | 1.00 30.07 | W | 0 |

^aAmino acids residues of the light (L) and heavy (H) chains are numbered according to the Chothia numbering system as shown in Tables 6 and 7, respectively (Al-Lazikani *et al., Jour. Mol. Biol.* 273:927-948, 1997). Amino acid residues of IL-13 (I) are numbered as shown in SEQ ID NO:4 (FIG. 2B). 30

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^bColumns are labeled according to Protein Data Bank Format, Version 2.2

Table 12. Structure coordinates of human IL-13/mAb13.2 Fab/IL-13Ra1a, b

| | Table 12 | • | struct | cure co | ordina | tes of huma | an 11-13 | /mAb13.2 | Fab/IL-I3Ral | | |
|----|--------------|----------|----------|----------------|----------|------------------|------------------|------------------|--------------------------|--------|----------|
| | | # | Name | Res. Cha | ain Res# | X | Y | \mathbf{z} | occ B | SegID | |
| | ATOM | 1 | СВ | PRO I | 6 | 27.016 | 30.544 | -8.876 | 1.00 78.94 | Ī | С |
| | ATOM | 2 | CG | PRO I | 6 | 25.927 | 30.356 | -7.827 | 1.00 79.11 | I | C |
| 5 | ATOM | 3 | C | PRO I | 6 | 28.494 | 28.571 | -9.333 | 1.00 77.04 | I | C |
| | ATOM | 4 | 0 | PRO I | 6 | 28.955 | 27.658 | -10.011 | 1.00 78.75 | I | 0 |
| | ATOM | 5 | N | PRO I | 6 | 26.037 | 28.388 | -9.357 | 1.00 79.03 | I | N |
| | ATOM | 6 | CD | PRO I | 6 | 25.355 | 28.902 | -8.177 | 1.00 78.57 | Ī | C |
| | MOTA | 7 | CA | PRO I | 6 | 27.169 | 29.250 | -9.667 | 1.00 77.81 | I | C |
| 10 | ATOM | 8 | N | SER I | 7 | 29.158 | 29.102 | -8.292 -7.754 | 1.00 73.92 1.00 70.46 | I | N C |
| | ATOM | 9 | CA | SER I | 7 | 30.314 31.594 | 28.399 28.866 | -7.754 -8.450 | 1.00 70.46 | I | C |
| | ATOM ATOM | 10 11 | CB OG | SER I SER I | 7 7 | 32.433 | 27.732 | -8.694 | 1.00 71.08 | Ï | Ö |
| | ATOM | 12 | C | SER I | 7 | 30.438 | 28.627 | -6.254 | 1.00 68.57 | Ï | č |
| 15 | ATOM | 13 | ŏ | SER I | ż | 29.807 | 29.505 | -5.678 | 1.00 68.82 | Ī | ŏ |
| | ATOM | 14 | Ň | THR I | 8 | 31.238 | 27.760 | -5.628 | 1.00 64.85 | I | N |
| | ATOM | 15 | CA | THR I | 8 | 31.542 | 27.924 | -4.220 | 1.00 61.35 | I | C |
| | ATOM | 16 | CB | THR I | 8 | 31.055 | 26.659 | -3.518 | 1.00 60.21 | I | C |
| | MOTA | 17 | OG1 | THR I | 8 | 31.602 | 25.526 | -4.191 | 1.00 60.16 | I | 0 |
| 20 | ATOM | 18 | CG2 | THR I | 8 | 29.525 | 26.585 | -3.602 | 1.00 60.47 | Ī | C |
| | ATOM | 19 | C | THR I | 8 | 33.049 | 28.098 | -4.021 | 1.00 59.39 | Ĭ | C |
| | ATOM | 20 | 0 | THR I | 8 | 33.866 | 27.692 | -4.837 | 1.00 60.36 | I | O |
| | ATOM | 21 | N | ALA I | 9 | 33.455 | 28.703 28.844 | -2.891 -2.652 | 1.00 56.29 1.00 53.24 | I | C N |
| OF | MOTA | 22 | CA CB | ALA I ALA I | 9 9 | 34.886 35.099 | 29.365 | -2.632 -1.233 | 1.00 53.24 | Ī | Č |
| 25 | ATOM ATOM | 23 24 | CD | ALA I | 9 | 35.601 | 27.499 | -2.836 | 1.00 50.08 | Ī | č |
| | ATOM | 25 | Õ | ALA I | 9 | 36.740 | 27.420 | -3.303 | 1.00 48.77 | Ī | ŏ |
| | ATOM | 26 | N | LEU I | 10 | 34.896 | 26.425 | -2.407 | 1.00 47.48 | I | N |
| | ATOM | 27 | CA | LEU I | 10 | 35.458 | 25.082 | -2.467 | 1.00 47.12 | I | C |
| 30 | ATOM | 28 | CB | LEU I | 10 | 34.532 | 24.133 | -1.702 | 1.00 47.12 | I | C |
| | MOTA | 29 | CG | LEU I | 10 | 35.161 | 22.751 | -1.483 | 1.00 47.82 | I | C |
| | MOTA | 30 | | LEU I | 10 | 36.663 | 22.837 | -1.178 | 1.00 46.75 | Ī | C |
| | MOTA | 31 | | LEU I | 10 | 34.533 | 21.987 | -0.316 | 1.00 47.41 | I | C, |
| | ATOM | 32 | C | LEU I | 10 | 35.641 | 24.597 | -3.910 | 1.00 45.94 | I | O. G. |
| 35 | ATOM | 33 | O | LEU I | 10 | 36.703 | 24.136 24.643 | -4.306 -4.689 | 1.00 44.31 1.00 45.74 | I | И |
| | MOTA MOTA | 34 35 | N CA | ARG I | 11 11 | 34.544 34.605 | 24.150 | -6.058 | 1.00 47.06 | Ï | C |
| | ATOM | 36 | CB | ARG I | 11 | 33.268 | 24.453 | -6.736 | 1.00 50.47 | Î | Č |
| | ATOM | 37 | CG | ARG I | 11 | 33.168 | 23.828 | -8.127 | 1.00 55.23 | Ī | Č |
| 40 | ATOM | 38 | CD | ARG I | 11 | 32.056 | 24.466 | -8.967 | 1.00 59.66 | I | C |
| | ATOM | 39 | NE | ARG I | 11 | 32.248 | 24.165 | -10.388 | 1.00 64.26 | I | N |
| | MOTA | 40 | CZ | ARG I | 11 | 31.352 | 23.350 | -10.973 | 1.00 67.01 | I | С |
| | MOTA | 41 | NH1 | | 11 | 30.187 | 23.118 | -10.391 | 1.00 67.52 | I | N |
| | MOTA | 42 | | ARG I | 11 | 31.638 | 22.791 | -12.151 | 1.00 66.67 | Ī | N |
| 45 | ATOM | 43 | C | ARG I | 11 | 35.750 | 24.793 | -6.845 | 1.00 46.55 | I | C |
| | ATOM | 44 | 0 | ARG I | 11 | 36.517 | 24.134 26.135 | -7.533 -6.761 | 1.00 47.11 1.00 46.28 | I I | N O |
| | MOTA | 45 | N | GLU I | 12 12 | 35.823 36.863 | 26.133 | -7.497 | 1.00 45.28 | I | C |
| | ATOM ATOM | 46 47 | CA CB | GLU I | | 36.654 | 28.346 | -7.313 | 1.00 46.38 | Ï | Č |
| 50 | ATOM | 48 | CG | GLU I | 12 | 35.298 | 28.819 | -7.850 | 1.00 49.26 | Ī | Č |
| 00 | ATOM | 49 | CD | GLU I | | 35.349 | 28.900 | -9.359 | 1.00 51.60 | I | C |
| | ATOM | 50 | | GLU I | | 36.412 | 29.179 | -9.898 | 1.00 54.40 | I | 0 |
| | ATOM | 51 | OE2 | GLU I | | 34.312 | 28.700 | -9.988 | 1.00 53.81 | I | 0 |
| | ATOM | 52 | C | GLU I | | 38.261 | 26.436 | -7.031 | 1.00 43.95 | I | C |
| 55 | MOTA | 53 | О | GLU I | | 39.205 | 26.341 | -7.804 | 1.00 44.02 | Ī | 0 |
| | ATOM | 54 | | LEU I | | 38.395 | 26.233 | -5.707 | 1.00 43.03 | I | N |
| | ATOM | 55 | | LEU I | | 39.685 | 25.790 | -5.186 | 1.00 43.21 | I | C |
| | MOTA | 56 | | LEU I | | 39.623 | 25.788 25.240 | -3.657 -3.027 | 1.00 41.91 1.00 43.10 | I | C |
| 60 | ATOM | 57 58 | | LEU I LEU I | | 40.902 42.136 | 26.054 | -3.419 | 1.00 40.08 | I | Č |
| 60 | MOTA MOTA | 59 | | | | 40.855 | 25.238 | -1.496 | 1.00 43.85 | Ī | C |
| | ATOM | 60 | | LEU I | | 40.035 | 24.389 | -5.688 | 1.00 44.05 | Ī | Č |
| | ATOM | 61 | | LEU I | | 41.146 | 24.103 | -6.105 | 1.00 44.32 | Ī | ō |
| | ATOM | 62 | | ILE I | | 39.045 | 23.485 | -5.597 | 1.00 44.06 | I | N |
| 65 | ATOM | 63 | | ILE I | | 39.276 | 22.125 | -6.074 | 1.00 44.78 | I | C |
| | ATOM | 64 | CB | ILE I | 14 | 37.978 | 21.332 | -5.907 | 1.00 42.05 | I | C |
| | MOTA | 65 | | ILE I | | 38.090 | 19.996 | -6.653 | 1.00 41.67 | Ī | C |
| | ATOM | 66 | CG1 | ILE I | 14 | 37.731 | 21.022 | -4.430 | 1.00 39.88 | I | С |

| | | | | | | 24 224 | | | | |
|----|--------------|------------|-----------|----------------|----------|------------------|----------------------------------|--------------------------|--------|--------|
| | ATOM | 68 | С | ILE I | 14 | 36.371 39.708 | | 1.00 38.79 | I | |
| | ATOM | 69 | ŏ | ILE I | 14 | 40.558 | | 1.00 47.20 1.00 47.59 | I | C |
| | ATOM | 70 | N | GLU I | 15 | 39.070 | | 1.00 47.59 | I I | O |
| 5 | MOTA | 71 | CA | GLU I | 15 | 39.369 | 23.015 -9.761 | 1.00 51.76 | Ī | N C |
| | ATOM | 72 | CB | GLU I | 15 | 38.372 | 23.943 -10.458 | 1.00 53.36 | Ī | Č |
| | ATOM | 73 | CG | GLU I | 15 | 36.969 | | 1.00 57.81 | Ī | č |
| | ATOM | 74 | CD | GLU I | 15 | 36.115 | | 1.00 61.60 | I | C |
| 10 | ATOM ATOM | 75 76 | OE1 | GLU I | 15 | 34.896 | | 1.00 63.74 | I | 0 |
| 10 | ATOM | 75 77 | C C | GLU I GLU I | 15 15 | 36.676 | 24.698 -12.394 | 1.00 64.24 | I | 0 |
| | ATOM | 78 | Ö | GLU I | 15 | 40.814 41.514 | 23.434 -10.041 22.839 -10.850 | 1.00 52.17 | Ī | C |
| | ATOM | 79 | N | GLU I | 16 | 41.252 | 22.839 -10.850 24.510 -9.359 | 1.00 53.33 | I | 0 |
| | ATOM | 80 | CA | GLU I | 16 | 42.665 | 24.891 -9.466 | 1.00 52.90 1.00 52.55 | I | N |
| 15 | MOTA | 81 | CB | GLU I | 16 | 42.895 | 26.165 -8.650 | 1.00 53.39 | I | C |
| | MOTA | 82 | CG | GLU I | 16 | 44.384 | 26.475 -8.463 | 1.00 54.58 | Ī | C |
| | ATOM | 83 | CD | GLU I | 16 | 44.954 | 27.031 -9.751 | 1.00 56.47 | Ī | č |
| | ATOM | 84 | | GLU I | 16 | 44.255 | 27.022 -10.754 | 1.00 56.93 | I | Ō |
| 20 | ATOM ATOM | 85 86 | OE2 | | 16 | 46.105 | 27.467 -9.741 | 1.00 56.71 | I | 0 |
| 20 | ATOM | 87 | C O | GLU I | 16 16 | 43.630 | 23.796 -9.001 | 1.00 51.84 | I | С |
| | ATOM | 88 | И | LEU I | 17 | 44.655 43.323 | 23.523 -9.623 23.187 -7.842 | 1.00 50.16 | Ī | 0 |
| | ATOM | 89 | CA | LEU I | 17 | 44.193 | 23.187 -7.842 22.107 -7.389 | 1.00 53.85 1.00 54.85 | I | N |
| | ATOM | 90 | СВ | LEU I | 17 | 43.658 | 21.562 -6.071 | 1.00 55.53 | I | C C |
| 25 | MOTA | 91 | CG | LEU I | 17 | 43.933 | 22.504 -4.894 | 1.00 57.93 | Ī | G |
| | MOTA | 92 | | LEU I | 17 | 43.907 | 21.778 -3.551 | 1.00 58.04 | Ī | Č |
| | ATOM | 93 | | LEU I | 17 | 45.303 | 23.190 -4.990 | 1.00 55.21 | Ī | č |
| | ATOM | 94 | C | LEU I | 17 | 44.287 | 20.988 -8.437 | 1.00 54.64 | I | C |
| 30 | ATOM ATOM | 95 96 | O | LEU I | 17 | 45.326 | 20.369 -8.649 | 1.00 53.29 | I | 0 |
| 00 | ATOM | 97 | N CA | VAL I VAL I | 18 18 | 43.134 43.143 | 20.699 -9.068 | 1.00 54.67 | I | N |
| | ATOM | 98 | CB | VAL I | 18 | 43.143 41.707 | 19.739 -10.170 19.562 -10.669 | 1.00 56.02 | I | C |
| | ATOM | 99 | | VAL I | 18 | 41.691 | 18.686 -11.919 | 1.00 55.67 1.00 54.36 | Ī | C |
| | ATOM | 100 | | VAL I | 18 | 40.855 | 18.904 -9.603 | 1.00 54.36 | I | C |
| 35 | MOTA | 101 | C | VAL I | 18 | 44.016 | 20.241 -11.309 | 1.00 56.81 | Ī | C |
| | MOTA | 102 | 0 | VAL I | 18 | 44.779 | 19.508 -11.927 | 1.00 56.49 | Ī | Ö |
| | MOTA | 103 | N | ASN I | 19 | 43.865 | 21.537 -11.615 | 1.00 58.66 | Ī | N |
| | ATOM | 104 | CA | ASN I | 19 | 44.587 | 22.072 -12.767 | 1.00 60.24 | I | C |
| 40 | ATOM | 105 | CB | ASN I | 19 | 44.243 | 23.553 -12.930 | 1.00 62.77 | I | C |
| 40 | ATOM ATOM | 106 107 | CG OD1 | ASN I ASN I | 19 19 | 44.463 | 23.973 -14.361 | 1.00 66.30 | I | С |
| | ATOM | 108 | | ASN I | 19 | 45.444 43.491 | 24.637 -14.697 23.599 -15.222 | 1.00 66.87 | Ī | 0 |
| | ATOM | 109 | C | ASN I | 19 | 46.106 | 21.874 -12.654 | 1.00 69.04 1.00 60.76 | Ī | N |
| | ATOM | 110 | Ö | ASN I | 19 | 46.760 | 21.386 -13.559 | 1.00 60.76 | I | C |
| 45 | ATOM | 111 | N | ILE I | 20 | 46.681 | 22.301 -11.506 | 1.00 60.66 | I | И |
| | MOTA | 112 | CA | ILE I | 20 | 48.133 | 22.233 -11.369 | 1.00 61.31 | Ī | Ĉ |
| | ATOM | 113 | CB | ILE I | 20 | 48.598 | 23.170 -10.239 | 1.00 59.89 | Ī | č |
| | ATOM | 114 | | ILE I | 20 | 48.081 | 24.601 -10.471 | 1.00 59.08 | I | C |
| 50 | ATOM ATOM | 115 116 | | ILE I | 20 | 48.081 | 22.695 -8.882 | 1.00 58.35 | I | С |
| 00 | ATOM | 117 | CDI | ILE I | 20 20 | 48.507 48.665 | 23.649 -7.757 20.804 -11.140 | 1.00 53.99 | Ī | C |
| | ATOM | 118 | ŏ | ILE I | 20 | 49.846 | 20.527 -11.286 | 1.00 62.24 | I | C |
| | ATOM | 119 | N | THR I | 21 | 47.766 | 19.884 -10.725 | 1.00 62.82 1.00 64.13 | I I | N O |
| | ATOM | 120 | CA | THR I | 21 | 48.272 | 18.536 -10.475 | 1.00 67.05 | Ī | C |
| 55 | ATOM | 121 | CB | THR I | 21 | 47.515 | 17.934 -9.292 | 1.00 65.01 | Ī | Č |
| | ATOM | 122 | | | 21 | 46.110 | 18.119 -9.493 | 1.00 65.20 | Ī | ŏ |
| | ATOM | 123 | | THR I | 21 | 47.934 | 18.634 -7.998 | 1.00 64.13 | I | Ċ |
| | ATOM | 124 | C | THR I | 21 | 48.149 | 17.601 -11.686 | 1.00 69.94 | I | С |
| 60 | ATOM ATOM | 125 126 | O | THR I | 21 | 48.386 | 16.404 -11.597 | 1.00 70.16 | I | 0 |
| 50 | ATOM | 127 | | GLN I GLN I | 22 22 | 47.717 47.796 | 18.156 -12.833 | 1.00 74.84 | Ī | N |
| | ATOM | 128 | | GLN I | 22 | 47.796 | 17.344 -14.039 18.242 -15.257 | 1.00 79.56 | Ī | C |
| | ATOM | 129 | | GLN I | 22 | 46.107 | 18.696 -15.411 | 1.00 79.69 1.00 82.15 | I | C |
| | ATOM | 130 | | GLN I | 22 | 46.038 | 19.891 -16.340 | 1.00 82.15 | I | C |
| 65 | MOTA | 131 | | GLN I | 22 | 46.743 | 20.011 -17.331 | 1.00 85.68 | I | 0 |
| | ATOM | 132 | NE2 | GLN I | 22 | 45.095 | 20.790 -15.993 | 1.00 84.96 | Ī | N |
| | ATOM | 133 | | GLN I | 22 | 49.182 | 16.717 -14.144 | 1.00 82.23 | Ī | Ĉ |
| | ATOM | 134 | | GLN I | 22 | 50.208 | 17.384 -14.054 | 1.00 82.99 | I | ō |
| | MOTA | 135 | N | ASN I | 23 | 49.204 | 15.378 -14.279 | 1.00 85.10 | I | N |

| | A TOM | 136 | CA | ASN I | 23 | 50.502 | 14.740 | -14.456 | 1.00 87.69 | I | С |
|-----|--------|-----|------------------|------------------------|----|--------|--------|---------|------------|-----|-----|
| | ATOM | | CA | | | | 13.225 | | 1.00 89.46 | Ī | č |
| | MOTA | 137 | СВ | ASN I | 23 | 50.318 | | | | | |
| | ATOM | 138 | CG | ASN I | 23 | 49.344 | 12.907 | | 1.00 91.98 | I | C |
| | MOTA | 139 | OD1 | ASN I | 23 | 48.554 | 13.754 | | 1.00 93.28 | I | 0 |
| 5 | MOTA | 140 | ND2 | ASN I | 23 | 49.394 | 11.647 | -16.047 | 1.00 92.89 | I | N |
| • | ATOM | 141 | C | ASN I | 23 | 51.177 | 15,233 | | 1.00 88.20 | I | C |
| | | | | ASN I | 23 | 52.391 | | -15.826 | 1.00 88.08 | Ī | ō |
| | MOTA | 142 | 0 | | | | | | | | |
| | MOTA | 143 | N | ASN I | 24 | 50.337 | 15.517 | -16./46 | 1.00 88.98 | I | N |
| | MOTA | 144 | $^{\rm CA}$ | ASN I | 24 | 50.868 | 16.147 | | 1.00 89.45 | I | C |
| 10 | MOTA | 145 | CB | ASN I | 24 | 49.697 | 16.736 | -18.743 | 1.00 89.76 | I | С |
| | ATOM | 146 | CG | ASN I | 24 | 48.615 | 15.708 | | 1.00 90.73 | I | С |
| | | | | ASN I | 24 | 47.436 | 16.026 | | 1.00 91.03 | I | Ō |
| | ATOM | 147 | | | | | | | | | |
| | ATOM | 148 | | ASN I | 24 | 49.058 | 14.445 | | 1.00 90.98 | I | N |
| | ATOM | 149 | С | ASN I | 24 | 51.783 | 17.295 | -17.596 | 1.00 89.22 | . I | С |
| 15 | ATOM | 150 | 0 | ASN I | 24 | 52.769 | 17.586 | -18.259 | 1.00 89.67 | I | 0 |
| | ATOM | 151 | N | LYS I | 25 | 51.384 | 18.011 | | 1.00 88.77 | I | N |
| | | | | | | 52.011 | | -16.317 | 1.00 88.13 | Ī | Ċ |
| | ATOM | 152 | CA | LYS I | 25 | | | | | | |
| | ATOM | 153 | СВ | LYS I | 25 | 51.236 | | -15.261 | 1.00 87.83 | I | |
| | ATOM | 154 | CG | LYS I | 25 | 50.573 | 21.287 | -15.901 | 1.00 88.09 | I | |
| 20 | ATOM | 155 | CD | LYS I | 25 | 49.298 | 21.716 | -15.180 | 1.00 87.96 | I | C |
| | MOTA | 156 | CE | LYS I | 25 | 48.765 | 23.021 | -15.758 | 1.00 87.47 | I | С |
| | | 157 | | LYS I | 25 | 47.511 | | -15.112 | 1.00 87.86 | I | |
| | ATOM | | \widetilde{NZ} | | | | | | 1.00 87.88 | Ī | |
| | ATOM | 158 | C | LYS I | 25 | 53.479 | | -15.941 | | | |
| | ATOM | 159 | 0 | LYS I | 25 | 54.359 | 19.464 | -16.732 | 1.00 87.93 | I | |
| 25 | MOTA | 160 | N | ALA I | 26 | 53.727 | 18.768 | -14.680 | 1.00 87.24 | I | |
| | MOTA | 161 | CA | ALA I | 26 | 55.097 | 18.639 | -14.190 | 1.00 87.03 | I | C |
| | ATOM | 162 | CB | ALA I | 26 | 55.920 | | -14.793 | 1.00 86.82 | I | C |
| | | | | | | 55.156 | | -12.659 | 1.00 86.17 | Ī | |
| | ATOM | 163 | C | ALA I | 26 | | | | | | |
| | ATOM | 164 | 0 | ALA I | 26 | 54.261 | | -12.003 | 1.00 86.49 | I | |
| 30 | ATOM | 165 | N | PRO I | 27 | 56.230 | 18.158 | -12.104 | 1.00 85.00 | I | |
| | ATOM | 166 | $^{\rm CD}$ | PRO I | 27 | 57.357 | 17.502 | -12.756 | 1.00 84.74 | I | С |
| | ATOM | 167 | CA | PRO I | 27 | 56.407 | 18.123 | -10.655 | 1.00 83.68 | I | C |
| | | | | | 27 | 57.843 | | -10.383 | 1.00 84.54 | Ī | |
| | MOTA | 168 | CB | PRO I | | | | | | Ī | |
| | ATOM | 169 | CG | PRO I | 27 | 58.352 | | -11.621 | 1.00 85.05 | | |
| 35 | ATOM | 170 | C | PRO I | 27 | 56.115 | | -10.015 | 1.00 82.78 | I | |
| | ATOM | 171 | 0 | PRO I | 27 | 56.807 | 20.461 | -10.226 | 1.00 82.59 | I | 0 |
| | ATOM | 172 | N | LEU I | 28 | 55.012 | 19.496 | -9.237 | 1.00 81.31 | I | N |
| | | 173 | CA | LEU I | 28 | 54.588 | 20.743 | -8.605 | 1.00 79.53 | I | |
| | ATOM | | | | | | | -7.864 | 1.00 79.22 | Ī | |
| | MOTA | 174 | СВ | LEU I | 28 | 53.272 | 20.461 | | | | |
| 40 | ATOM | 175 | CG | LEU I | 28 | 52.572 | 21.747 | -7.428 | 1.00 78.56 | I | |
| | MOTA | 176 | CD1 | LEU I | 28 | 52.267 | 22.680 | -8.604 | 1.00 79.42 | I | |
| | ATOM | 177 | CD2 | LEU I | 28 | 51.238 | 21.483 | -6.732 | 1.00 78.52 | I | C |
| | ATOM | 178 | C | LEU I | 28 | 55.648 | 21.319 | -7.638 | 1.00 78.97 | I | |
| | | | | LEU I | 28 | 55.966 | 20.770 | -6.599 | 1.00 78.25 | Ī | |
| | MOTA | 179 | 0 | | | | | | | Ī | |
| 45 | MOTA | 180 | N | CYS I | 29 | 56.233 | 22.451 | -8.080 | 1.00 78.37 | | |
| | MOTA | 181 | $^{\rm CA}$ | CYS I | 29 | 57.063 | 23.311 | -7.222 | 1.00 78.80 | I | _ |
| | MOTA | 182 | С | CYS I | 29 | 58.558 | 22.927 | -7.126 | 1.00 79.64 | I | С |
| | MOTA | 183 | 0 | CYS I | 29 | 59.399 | 23.724 | -6.710 | 1.00 81.19 | I | 0 |
| | MOTA | 184 | ČВ | CYS I | 29 | 56.387 | 23.648 | -5.869 | 1.00 78.02 | I | |
| | | | | | | 55.321 | 25.110 | -5.991 | 1.00 79.53 | Ī | |
| 50 | MOTA | 185 | SG | CYS I | 29 | | | | | | |
| | MOTA | 186 | N | ALA I | 30 | 58.833 | 21.638 | -7.488 | 1.00 79.61 | I | |
| | MOTA | 187 | $^{\rm CA}$ | ALA I | 30 | 60.144 | 21.242 | -8.025 | 1.00 79.88 | I | |
| | MOTA | 188 | CB | ALA I | 30 | 60.819 | 22.492 | -8.580 | 1.00 79.91 | I | C |
| | MOTA | 189 | C | ALA I | 30 | 61.080 | 20.547 | -7.032 | 1.00 79.67 | I | |
| | | | | | | 62.298 | 20.718 | -7.049 | 1.00 80.11 | Ī | |
| 55 | MOTA | 190 | 0 | ALA I | 30 | | | | | | |
| | MOTA | 191 | N | GLY I | 31 | 60.482 | 19.717 | -6.179 | 1.00 79.21 | I | |
| | ATOM | 192 | $^{\rm CA}$ | GLY I | 31 | 61.112 | 19.428 | -4.906 | 1.00 79.39 | I | |
| | ATOM | 193 | С | GLY I | 31 | 60.344 | 20.181 | -3.821 | 1.00 78.91 | I | C |
| | ATOM | 194 | ŏ | GLY I | 31 | 59.220 | 19.845 | -3.484 | 1.00 80.31 | I | |
| 60 | | | | | | 60.988 | 21.238 | -3.271 | 1.00 77.08 | Ī | |
| 60 | ATOM | 195 | N | SER I | 32 | | | | | | |
| | MOTA | 196 | ca | SER I | 32 | 60.317 | 22.073 | -2.255 | 1.00 75.27 | I | |
| | ATOM | 197 | CB | SER I | 32 | 59.382 | 23.064 | -2.969 | 1.00 76.77 | I | |
| | MOTA | 198 | OG | SER I | 32 | 60.013 | 24.342 | -3.017 | 1.00 80.23 | I | |
| | ATOM | 199 | Ċ | SER I | 32 | 59.517 | 21.252 | -1.233 | 1.00 73.51 | I | |
| GF. | | 200 | | SER I | 32 | 58.519 | 20.628 | -1.553 | 1.00 73.95 | Ī | |
| 65 | ATOM | | 0 | | | | | | 1.00 71.50 | I | |
| | MOTA | 201 | N | MET I | 33 | 59.990 | 21.253 | 0.035 | | | |
| | ATOM | 202 | CA | MET I | 33 | 59.323 | 20.420 | 1.043 | 1.00 68.96 | I | |
| | MOTA | 203 | CB | MET I | 33 | 60.384 | 19.555 | 1.713 | 1.00 69.85 | I | |
| | ATOM | 204 | CG | MET I | 33 | 61.259 | 18.852 | 0.686 | 1.00 70.72 | 1 | : C |
| | 111011 | | | | | | | | | | |

| | ATOM ATOM | 205 206 | SD MET I CE MET I | 33 33 | 60.793 61.652 | 17.138 16.452 | 0.458 1.874 | 1.00 73.74 1.00 72.51 | I | s C |
|----|--------------|---|------------------------|----------|-------------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM ATOM | 207 208 | C MET I O MET I | 33 33 | 58.580 59.084 | 21.248 22.195 | 2.085 2.664 | 1.00 66.87 1.00 67.96 | I | C |
| 5 | ATOM | 209 | N VAL I | 34 | 57.293 | 20.874 | 2.281 | 1.00 64.12 | I | N |
| | MOTA | 210 | CA VAL I | 34 | 56.489 | 21.588 | 3.270 | 1.00 62.22 | I | C |
| | ATOM | $\begin{array}{c} 211 \\ 212 \end{array}$ | CB VAL I CG1 VAL I | 34 34 | 55.262 55.684 | 22.183 23.296 | 2.578 1.626 | 1.00 62.02 1.00 60.10 | I | C |
| | ATOM ATOM | 213 | CG2 VAL I | 34 | 54.532 | 21.107 | 1.800 | 1.00 58.25 | Ī | č |
| 10 | ATOM | 214 | C VAL I | 34 | 56.029 | 20.700 | 4.450 | 1.00 62.11 | I | C |
| | MOTA | 215 | O VAL I | 34 | 56.054 | 19.479 21.355 | 4.372 5.548 | 1.00 61.47 1.00 61.68 | I | N O |
| | ATOM ATOM | 216 217 | N TRP I CA TRP I | 35 35 | 55.618 55.103 | 20.602 | 6.682 | 1.00 62.60 | İ | Ç |
| | ATOM | 218 | CB TRP I | 35 | 54.958 | 21.567 | 7.862 | 1.00 63.98 | I | C |
| 15 | MOTA | 219 | CG TRP I | 35 | 56.272 | 22.146 | 8.225 | 1.00 66.88 | I | C |
| | MOTA MOTA | 220 221 | CD2 TRP I CE2 TRP I | 35 35 | 57.297 58.343 | 21.517 22.460 | 9.027 9.190 | 1.00 67.70 1.00 68.28 | Ì | C |
| | ATOM | 222 | CEZ TRP I | 35 | 57.413 | 20.260 | 9.614 | 1.00 68.19 | Ī | С |
| | MOTA | 223 | CD1 TRP I | 35 | 56.738 | 23.441 | 7.917 | 1.00 66.99 | I | C |
| 20 | ATOM ATOM | 224 225 | NE1 TRP I CZ2 TRP I | 35 35 | 57.957 59.461 | 23.700 22.131 | $8.466 \\ 9.942$ | 1.00 67.36 1.00 69.16 | I | N C |
| | ATOM | 226 | CZ3 TRP I | 35 | 58.531 | 19.930 | 10.361 | 1.00 68.91 | I | С |
| | ATOM | 227 | CH2 TRP I | 35 | 59.566 | 20.873 | 10.520 | 1.00 69.23 | I | C |
| 25 | ATOM ATOM | 228 229 | C TRP I O TRP I | 35 35 | 53.742 52.840 | 19.994 20.652 | 6.356 5.855 | 1.00 62.37 1.00 62.15 | I | C O |
| 25 | ATOM | 230 | N SER I | 36 | 53.617 | 18.680 | 6.609 | 1.00 61.20 | Ĩ | N |
| | ATOM | 231 | CA SER I | 36 | 52.275 | 18.095 | 6.574 | 1.00 61.84 | Ī | C |
| | ATOM ATOM | 232 233 | CB SER I OG SER I | 36 36 | 52.414 52.742 | 16.571 16.233 | 6.702 8.048 | 1.00 62.31 1.00 65.85 | I | C |
| 30 | ATOM | 234 | C SER I | 36 | 51.383 | 18.640 | 7.689 | 1.00 60.45 | I | C |
| | MOTA | 235 | O SER I | 36 | 51.831 | 19.023 | 8.763 | 1.00 60.13 | I | 0 |
| | ATOM ATOM | 236 237 | N ILE I CA ILE I | 37 37 | 50.069 49.138 | 18.705 19.284 | 7.388 8.348 | 1.00 60.87 1.00 62.76 | I | N N |
| | ATOM | 238 | CB ILE I | 37 | 48.525 | 20.527 | 7.703 | 1.00 60.98 | I. | C |
| 35 | MOTA | 239 | CG2 ILE I | 37 | 49.641 | 21.486 | 7.246 | 1.00 60.58 | Ī | C |
| | ATOM ATOM | $\frac{240}{241}$ | CG1 ILE I CD1 ILE I | 37 37 | 47.726 46.656 | 20.118 21.150 | 6.461 6.106 | 1.00 61.47 1.00 63.20 | I | C |
| | ATOM | 242 | C ILE I | 37 | 48.015 | 18.316 | 8.735 | 1.00 64.55 | Ī | С |
| | MOTA | 243 | O ILE I | 37 | 47.844 | 17.247 | 8.163 | 1.00 64.40 | I | 0 |
| 40 | ATOM ATOM | 244 245 | N ASN I CA ASN I | 38 38 | 47.249 46.117 | 18.723 17.915 | 9.757 10.192 | 1.00 67.19 1.00 69.16 | I I | C N |
| ĺ | ATOM | 245 | CB ASN I | 38 | 45.872 | 18.200 | 11.675 | 1.00 71.48 | Ī | C |
| | MOTA | 247 | CG ASN I | 38 | 46.010 | 16.925 | 12.468 | 1.00 74.53 | I | C |
| 45 | ATOM ATOM | 248 249 | OD1 ASN I ND2 ASN I | 38 38 | 45.727 46.427 | 16.866 15.862 | 13.660 11.758 | 1.00 76.30 1.00 76.89 | I | N |
| 43 | MOTA | 250 | C ASN I | 38 | 44.853 | 18.237 | 9.387 | 1.00 70.38 | I | , C |
| | MOTA | 251 | O ASN I | 38 | 44.318 | 19.337 | 9.422 | 1.00 70.94 | I | O |
| | ATOM ATOM | 252 253 | N LEU I CA LEU I | 39 39 | 44.401 43.191 | 17.230 17.403 | 8.613 7.817 | 1.00 71.67 1.00 73.26 | I | N C |
| 50 | MOTA | 254 | CB LEU I | 39 | 43.216 | 16.369 | 6.691 | 1.00 71.42 | I | С |
| | MOTA | 255 | CG LEU I | 39 | 44.416 | 16.557 | 5.761 | 1.00 70.72 | I | C C |
| | ATOM ATOM | 256 257 | CD1 LEU I CD2 LEU I | 39 39 | 44.567 44.331 | 15.415 17.845 | $4.753 \\ 4.944$ | 1.00 69.87 1.00 68.56 | I | C |
| | ATOM | 258 | C LEU I | 39 | 41.924 | 17.225 | 8.662 | 1.00 74.76 | I | С |
| 55 | ATOM | 259 | O LEU I | 39 | 40.887 | 16.763 | 8.201 | 1.00 75.68 1.00 76.50 | I I | N O |
| | ATOM ATOM | 260 261 | N THR I CA THR I | 40 40 | $\frac{42.048}{40.904}$ | 17.574 17.441 | 9.956 10.850 | 1.00 78.30 | I | C |
| | ATOM | 262 | CB THR I | 40 | 41.422 | 17.074 | 12.241 | 1.00 78.89 | I | С |
| | ATOM | 263 | OG1 THR I | 40 | 40.752 | 17.875 | 13.216 | 1.00 80.37 | I | C O |
| 60 | MOTA MOTA | 264 265 | CG2 THR I | 40 40 | 42.926 40.086 | 17.345 18.734 | 12.328 10.919 | 1.00 80.30 1.00 78.70 | Ĭ | G |
| | ATOM | 266 | O THR I | 40 | 38.886 | 18.762 | 10.684 | 1.00 80.14 | I | 0 |
| | MOTA | 267 | N ALA I | 41 | 40.775 | 19.826 | 11.301 | 1.00 77.65 1.00 76.51 | I I | N C |
| 65 | ATOM ATOM | 268 269 | CA ALA I CB ALA I | 41 41 | 40.097 39.375 | 21.115 21.199 | 11.376 12.721 | 1.00 76.51 | I | C |
| 00 | ATOM | 270 | C ALA I | 41 | 41.083 | 22.276 | 11.238 | 1.00 75.39 | I | С |
| | ATOM | 271 | O ALA I | 41 | 42.295 | 22.105 23.491 | 11.220 11.101 | 1.00 76.85 1.00 72.26 | I | O N |
| | MOTA MOTA | 272 273 | N GLY I CA GLY I | 42 42 | 40.522 41.385 | 24.649 | 10.911 | 1.00 72.28 | Ī | C |
| | | | | | | | | | | |

| | ATOM ATOM ATOM | 274 C GLY I 42 275 O GLY I 42 276 N MET I 43 277 CA MET I 43 | 42.460 24.359 9.862 1.00 65.34 43.566 24.883 9.890 1.00 63.64 42.109 23.451 8.934 1.00 62.58 43.066 23.063 7.907 1.00 61.81 | I C I O I N I C |
|----|--------------------------------------|---|---|---------------------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 278 CB MET I 43 279 CG MET I 43 280 SD MET I 43 281 CE MET I 43 282 C MET I 43 | 42.560 21.786 7.235 1.00 64.31 42.556 21.887 5.709 1.00 67.10 40.973 21.412 5.002 1.00 73.29 41.014 22.487 3.561 1.00 70.95 43.264 24.166 6.865 1.00 58.78 | I C I S I C I C I C I O |
| 10 | ATOM ATOM ATOM ATOM ATOM | 283 O MET I 43 284 N TYR I 44 285 CA TYR I 44 286 CB TYR I 44 287 CG TYR I 44 | 44.344 24.362 6.323 1.00 59.66 42.164 24.878 6.554 1.00 54.94 42.293 25.974 5.602 1.00 50.88 40.996 26.785 5.604 1.00 51.73 40.009 26.173 4.671 1.00 51.67 40.411 25.757 3.403 1.00 51.08 | I N I C I C I C |
| 15 | ATOM ATOM ATOM ATOM ATOM | 288 CD1 TYR I 44 289 CE1 TYR I 44 290 CD2 TYR I 44 291 CE2 TYR I 44 292 CZ TYR I 44 | 39.505 25.139 2.552 1.00 51.62 38.687 25.980 5.071 1.00 51.42 37.779 25.371 4.217 1.00 52.73 38.183 24.952 2.963 1.00 53.13 | I C I C I C |
| 20 | ATOM ATOM ATOM ATOM ATOM | 293 OH TYR I 44 294 C TYR I 44 295 O TYR I 44 296 N CYS I 45 297 CA CYS I 45 | 37.296 24.302 2.126 1.00 54.49 43.479 26.869 5.967 1.00 48.15 44.371 27.131 5.170 1.00 45.25 43.454 27.370 7.216 1.00 48.39 44.568 28.192 7.674 1.00 49.37 45.863 27.379 7.767 1.00 49.62 | I C I C I C |
| 25 | ATOM ATOM ATOM ATOM ATOM | 298 C CYS I 45 299 O CYS I 45 300 CB CYS I 45 301 SG CYS I 45 302 N ALA I 46 | 46.953 27.854 7.477 1.00 48.36 44.212 28.771 9.046 1.00 51.15 42.721 29.792 8.999 1.00 56.43 45.720 26.119 8.223 1.00 49.15 46.898 25.272 8.376 1.00 47.97 | I O I C I S I N I C |
| 30 | ATOM ATOM ATOM ATOM ATOM | 303 CA ALA I 46 304 CB ALA I 46 305 C ALA I 46 306 O ALA I 46 307 N ALA I 47 | 46.475 23.966 9.051 1.00 47.77 47.575 24.978 7.032 1.00 47.47 48.792 24.976 6.904 1.00 47.08 46.743 24.679 6.016 1.00 45.70 47.304 24.448 4.690 1.00 46.29 | I C I C |
| 35 | MOTA ATOM ATOM ATOM ATOM | 308 CA ALA I 47 309 CB ALA I 47 310 C ALA I 47 311 O ALA I 47 312 N LEU I 48 | 46.187 23.965 3.764 1.00 44.99 47.937 25.724 4.131 1.00 46.25 48.926 25.704 3.410 1.00 46.92 47.298 26.864 4.459 1.00 45.80 | I C I O I N I C |
| 40 | ATOM ATOM ATOM ATOM ATOM | 313 CA LEU I 48 314 CB LEU I 48 315 CG LEU I 48 316 CD1 LEU I 48 317 CD2 LEU I 48 | 46.891 29.252 4.496 1.00 43.51 47.494 30.657 4.381 1.00 42.29 47.729 31.076 2.928 1.00 39.28 46.606 31.740 4.998 1.00 41.45 | I C I C I C I C |
| 45 | MOTA MOTA MOTA MOTA MOTA | 318 C LEU I 48 319 O LEU I 48 320 N GLU I 49 321 CA GLU I 49 322 CB GLU I 49 | 50.204 28.759 4.093 1.00 45.62 49.255 28.124 6.044 1.00 46.20 50.467 28.352 6.822 1.00 47.25 50.132 28.090 8.289 1.00 49.57 | I ON I C |
| 50 | ATOM ATOM ATOM ATOM ATOM | 323 CG GLU I 49 324 CD GLU I 49 325 OE1 GLU I 49 326 OE2 GLU I 49 327 C GLU I 49 | 50.461 30.375 9.167 1.00 54.88 51.143 30.341 10.181 1.00 58.35 50.587 31.239 8.300 1.00 53.85 51.617 27.442 6.388 1.00 48.23 | I C I O I C I |
| 55 | ATOM ATOM ATOM ATOM ATOM | 328 O GLU I 49 329 N SER I 50 330 CA SER I 50 331 CB SER I 50 332 OG SER I 50 | 51.255 26.371 5.662 1.00 48.38 52.363 25.494 5.298 1.00 48.77 51.909 24.047 5.493 1.00 49.02 52.793 23.175 4.786 1.00 49.21 | I N I C I O I C |
| 60 | MOTA MOTA MOTA MOTA MOTA | 333 C SER I 50 334 O SER I 50 335 N LEU I 51 336 CA LEU I 51 337 CB LEU I 51 338 CG LEU I 51 | 53.961 25.559 3.484 1.00 48.73 51.812 26.041 2.997 1.00 47.10 52.118 26.266 1.589 1.00 47.89 50.821 26.119 0.793 1.00 46.69 50.533 24.668 0.401 1.00 49.04 | I O I C I C |
| 65 | MOTA MOTA MOTA MOTA MOTA | 338 CG LEU I 51 339 CD1 LEU I 51 340 CD2 LEU I 51 341 C LEU I 51 342 O LEU I 51 | 49.442 24.556 -0.665 1.00 50.21 51.760 23.952 -0.165 1.00 46.43 52.712 27.658 1.358 1.00 48.63 53.188 27.996 0.282 1.00 48.41 | I C I O |

| | ATOM | 343 | N | ILE I | 52 | 52.637 | 28.491 | 2.413 | 1.00 49.30 | I | N |
|----|--------------|-------------------|-----------|----------------|----------|------------------|------------------|-----------------------|--------------------------|--------|---------|
| | ATOM | 344 | CA | ILE I | 52 | 53.124 | 29.859 | 2.285 3.419 | 1.00 50.61 1.00 49.79 | I I | C |
| | MOTA MOTA | 345 346 | CB CG2 | ILE I | 52 52 | 52.519 53.293 | 30.688 30.428 | $\frac{3.419}{4.724}$ | 1.00 49.21 | Ī | č |
| 5 | ATOM | 347 | CG1 | ILE I | 52 | 52.627 | 32.181 | 3.098 | 1.00 48.59 | I | C |
| _ | MOTA | 348 | CD1 | | 52 | 52.045 | 32.525 | 1.727 | 1.00 45.04 1.00 51.05 | I | C |
| | ATOM | 349 | C | ILE I ILE I | 52 52 | 54.652 55.268 | 29.931 30.958 | $2.341 \\ 2.087$ | 1.00 51.05 1.00 53.83 | Ï | Ö |
| | ATOM ATOM | 350 351 | N O | ASN I | 53 | 55.265 | 28.798 | 2.730 | 1.00 51.02 | I | N |
| 10 | MOTA | 352 | CA | ASN I | 53 | 56.720 | 28.765 | 2.818 | 1.00 51.33 | I | C |
| | MOTA | 353 | СВ | ASN I | 53 | 57.111 | 27.732 28.261 | 3.876 5.244 | 1.00 47.60 1.00 47.65 | I I | C |
| | ATOM ATOM | 354 355 | CG OD1 | ASN I ASN I | 53 53 | 56.768 57.029 | 29.413 | 5.578 | 1.00 47.83 | Ī | ŏ |
| | ATOM | 356 | | ASN I | 53 | 56.161 | 27.379 | 6.056 | 1.00 45.54 | I | N |
| 15 | MOTA | 357 | C | ASN I | 53 | 57.360 | 28.407 | 1.475 | 1.00 53.53 | I | C O |
| | ATOM | 358 | O | ASN I | 53 54 | 58.573 56.533 | 28.418 28.020 | 1.313 0.484 | 1.00 55.03 1.00 55.95 | I | N |
| | ATOM ATOM | 359 360 | N CA | VAL I VAL I | 54 54 | 57.100 | 27.653 | -0.810 | 1.00 57.77 | Ī | C |
| | ATOM | 361 | CB | VAL I | 54 | 55.997 | 27.031 | -1.665 | 1.00 56.62 | I | C |
| 20 | MOTA | 362 | | VAL I | 54 | 56.544 | 26.690 | -3.050 | 1.00 53.96 | I | C |
| | MOTA | 363 | CG2 | VAL I VAL I | 54 54 | 55.484 57.696 | 25.765 28.866 | -1.006 -1.528 | 1.00 57.42 1.00 59.21 | I | C |
| | ATOM ATOM | 364 365 | C O | VAL I | 54 54 | 57.025 | 29.846 | -1.826 | 1.00 60.15 | I | 0 |
| | ATOM | 366 | N | SER I | 55 | 59.016 | 28.790 | -1.772 | 1.00 60.64 | I | N |
| 25 | MOTA | 367 | CA | SER I | 55 | 59.701 | 29.918 30.076 | -2.390 -1.702 | 1.00 63.25 1.00 62.79 | I | C |
| | ATOM ATOM | 368 369 | CB OG | SER I SER I | 55 55 | 61.060 61.384 | 31.463 | -1.600 | 1.00 63.77 | Ī | ŏ |
| | MOTA | 370 | C | SER I | 55 | 59.902 | 29.717 | -3.895 | 1.00 63.87 | I | C |
| | ATOM | 371 | 0 | SER I | 55 | 60.192 | 28.631 | -4.378 | 1.00 64.14 | I | NO |
| 30 | ATOM | 372 | N | GLY I | 56 56 | 59.683 60.020 | 30.814 30.814 | -4.647 -6.068 | 1.00 65.44 1.00 67.00 | I | G 10 |
| | ATOM ATOM | 373 374 | CA C | GLY I | 56 | 59.271 | 29.742 | -6.869 | 1.00 67.92 | I | C |
| | ATOM | 375 | Ö | GLY I | 56 | 59.850 | 28.975 | -7.626 | 1.00 68.15 | Ī | 0 |
| | MOTA | 376 | N | CYS I | 57 | 57.942 | 29.687 | -6.661 -7.503 | 1.00 68.54 1.00 68.81 | I | С |
| 35 | ATOM ATOM | 377 378 | CA C | CYS I | 57 57 | 57.166 55.803 | 28.788 29.402 | -7.865 | 1.00 67.61 | Ī | C |
| | ATOM | 379 | Ö | CYS I | 57 57 | 55.028 | 29.826 | -7.003 | 1.00 66.76 | I | 0 |
| | ATOM | 380 | CB | CYS I | 57 | 56.999 | 27.498 | -6.693 | 1.00 70.76 | I | C S |
| 40 | MOTA | 381 | SG | CYS I SER I | 57 58 | 56.071 55.726 | 26.192 29.762 | -7.524 -9.162 | 1.00 75.77 1.00 65.88 | I I | N |
| 40 | ATOM ATOM | 382 383 | N CA | SER I | 58 | 54.578 | 30.538 | -9.626 | 1.00 65.26 | Ī | C |
| | ATOM | 384 | CB | SER I | 58 | 54.958 | 31.236 | -10.936 | 1.00 65.56 | I | C |
| | MOTA | 385 | OG | SER I | 58 50 | 55.073 53.319 | 30.270 29.687 | -11.982 -9.825 | 1.00 66.55 1.00 64.15 | I I | 0 |
| 45 | ATOM ATOM | 386 387 | C O | SER I SER I | 58 58 | 52.266 | 30.169 | -10.222 | 1.00 63.50 | Ī | ŏ |
| 40 | ATOM | 388 | N | ALA I | 59 | 53.455 | 28.375 | -9.562 | 1.00 62.82 | I | N |
| | MOTA | 389 | CA | ALA I | 59 | 52.326 | 27.484 | -9.813 | 1.00 62.09 1.00 61.09 | I | C |
| | MOTA MOTA | 390 391 | CB C | ALA I ALA I | 59 59 | 52.868 51.366 | 26.101 27.384 | -10.175 -8.621 | 1.00 62.03 | Ï | Č |
| 50 | ATOM | 392 | ŏ | ALA I | 59 | 50.187 | 27.091 | -8.765 | 1.00 61.38 | I | 0 |
| | ATOM | 393 | N | ILE I | 60 | 51.906 | 27.598 | -7.403 | 1.00 60.60 | I | N |
| | ATOM | 394 | CA | ILE I ILE I | 60 60 | 51.033 51.743 | 27.514 26.744 | -6.233 -5.117 | 1.00 61.29 1.00 62.02 | I | C |
| | ATOM ATOM | 395 396 | CB CG2 | | 60 | 51.743 | 25.284 | -5.096 | 1.00 61.63 | I | C |
| 55 | ATOM | 397 | CG1 | | | 53.256 | 26.741 | -5.334 | 1.00 62.92 | Ī | C |
| | MOTA | 398 | | l ILE I | | 53.948 | 27.890 | -4.598 5.721 | 1.00 65.77 1.00 60.92 | I | C |
| | ATOM | 399 | C O | ILE I ILE I | | 50.602 49.867 | 28.887 29.018 | -5.721 -4.752 | 1.00 60.92 | Ī | ŏ |
| | ATOM ATOM | $\frac{400}{401}$ | N | GLU I | | 51.112 | 29.943 | -6.377 | 1.00 60.36 | I | N |
| 60 | MOTA | 402 | CA | GLU I | 61 | 50.752 | 31.274 | -5.910 | 1.00 59.69 | I | C |
| | ATOM | 403 | CB | GLU I | | 51.397 | 32.318 33.217 | -6.823 -6.060 | 1.00 62.53 1.00 68.64 | I | C |
| | ATOM ATOM | 404 405 | CG CD | GLU I GLU I | | 52.373 52.334 | 34.612 | -6.640 | 1.00 08.04 | Ī | Č |
| | ATOM | 405 | OE: | | | 51.637 | 35.456 | -6.093 | 1.00 72.04 | I | 0 |
| 65 | MOTA | 407 | OE2 | 2 GLU I | 61 | 53.018 | 34.848 | -7.635 | 1.00 74.33 | I | С О |
| | MOTA | 408 | C | GLU I | | 49.231 48.677 | 31.460 31.954 | -5.849 -4.877 | 1.00 57.43 1.00 56.73 | I | 0 |
| | MOTA MOTA | 409 410 | N | LYS I | | 48.550 | 31.067 | -6.943 | 1.00 55.24 | I | N |
| | MOTA | 411 | CA | | | 47.096 | 31.204 | -6.956 | 1.00 54.11 | I | С |

| | ATOM | 412 | СВ | LYS I | 62 | 46.570 | 30.752 | -8.319 | 1.00 54.42 | I | С |
|----|--------------|------------|--------------|----------------|----------------|------------------|------------------|-------------------|--------------------------|---|--------|
| | ATOM | 413 | CG | LYS I | 62 | 45.070 | 31.016 | -8.470 | 1.00 55.70 | Ĭ | C |
| | MOTA | 414 | CD | LYS I | 62 | 44.591 43.078 | 30.848 30.621 | -9.912 -10.004 | 1.00 57.84 1.00 58.76 | I | C |
| 5 | ATOM ATOM | 415 416 | CE NZ | LYS I LYS I | 62 62 | 42.630 | | -11.379 | 1.00 59.46 | Ï | Ŋ |
| 5 | MOTA | 417 | C | LYS I | 62 | 46.431 | 30.389 | -5.842 | 1.00 51.70 | I | C |
| | ATOM | 418 | ō | LYS I | 62 | 45.442 | 30.790 | -5.243 | 1.00 51.21 | I | 0 |
| | ATOM | 419 | \mathbf{N} | THR I | 63 | 46.985 | 29.185 | -5.602 | 1.00 49.68 | I | N |
| | MOTA | 420 | CA | THR I | 63 | 46.452 | 28.355 | -4.525 | 1.00 49.40 1.00 49.66 | I | C |
| 10 | ATOM ATOM | 421 422 | CB OG1 | THR I | 63 63 | 47.196 46.853 | 27.021 26.299 | -4.530 -5.714 | 1.00 49.02 | Ī | ŏ |
| | ATOM | 423 | CG2 | | 63 | 46.782 | 26.192 | -3.310 | 1.00 48.32 | Ī | C |
| | ATOM | 424 | C | THR I | 63 | 46.625 | 29.037 | -3.168 | 1.00 49.94 | I | C |
| | ATOM | 425 | 0 | THR I | 63 | 45.750 | 29.030 | -2.312 | 1.00 49.16 | ī | 0 |
| 15 | ATOM | 426 | N | GLN I | 64 | 47.828 | 29.601 30.380 | -2.971 -1.766 | 1.00 50.00 1.00 49.18 | I | N N |
| | ATOM | 427 428 | CA CB | GLN I GLN I | 64 64 | 48.064 49.444 | 31.026 | -1.889 | 1.00 49.16 | Ī | č |
| | ATOM ATOM | 429 | CG | GLN I | 64 | 50.577 | 30.038 | -1.627 | 1.00 50.10 | Ī | Ĉ |
| | MOTA | 430 | CD | GLN I | 64 | 51.901 | 30.746 | -1.780 | 1.00 51.30 | I | C |
| 20 | MOTA | 431 | OE1 | | 64 | 52.056 | 31.717 | -2.504 | 1.00 53.24 | Ī | 0 |
| | MOTA | 432 | NE2 | | 64 | 52.891 | 30.211 31.469 | -1.040 -1.597 | 1.00 47.60 1.00 49.30 | I | N C |
| | ATOM ATOM | 433 434 | C | GLN I GLN I | 64 64 | 47.004 46.492 | 31.409 31.724 | -0.516 | 1.00 50.23 | Ī | ŏ |
| | ATOM | 435 | N | ARG I | 65 | 46.702 | 32.147 | -2.718 | 1.00 49.37 | I | N |
| 25 | ATOM | 436 | CA | ARG I | 65 | 45.771 | 33.263 | -2.639 | 1.00 49.52 | Ī | C |
| | ATOM | 437 | CB | ARG I | 65 | 45.892 | 34.095 | -3.919 | 1.00 52.37 | I | C |
| | ATOM | 438 | CG | ARG I | 65 65 | 47.116 47.199 | 35.013 35.977 | -3.869 -5.060 | 1.00 55.43 1.00 58.20 | Ī | Č |
| | ATOM ATOM | 439 440 | CD NE | ARG I ARG I | 65 | 47.732 | 37.273 | -4.625 | 1.00 61.26 | Ī | N |
| 30 | ATOM | 441 | CZ | ARG I | 65 | 49.032 | 37.535 | -4.870 | 1.00 60.37 | I | С |
| • | MOTA | 442 | | ARG I | 65 | 49.771 | 36.671 | -5.541 | 1.00 62.13 | Ī | N |
| | ATOM | 443 | NH2 | | 65 | 49.595 | 38.624 | -4.337 | 1.00 59.84 | I | N C |
| | ATOM | 444 | C | ARG I | 65 65 | 44.329 43.526 | 32.802 33.477 | -2.402 -1.771 | 1.00 47.23 1.00 46.87 | I | 0 |
| 35 | ATOM ATOM | 445 446 | N O | ARG I MET I | 66 | 43.996 | 31.620 | -2.951 | 1.00 45.98 | Ī | N |
| 33 | ATOM | 447 | CA | MET I | 66 | 42.650 | 31.105 | -2.732 | 1.00 45.22 | I | C |
| | ATOM | 448 | CB | MET I | 66 | 42.402 | 29.953 | -3.705 | 1.00 46.64 | I | C |
| | MOTA | 449 | CG | MET I | 66 | 42.429 | 30.420 | -5.162 | 1.00 48.54 1.00 52.12 | I | C S |
| 40 | MOTA | 450 | SD CE | MET I MET I | 66 66 | 42.132 40.419 | 29.076 29.463 | -6.318 -6.708 | 1.00 52.12 1.00 51.79 | I | C |
| 40 | MOTA MOTA | 451 452 | CE | MET I | 66 | 42.443 | 30.649 | -1.284 | 1.00 43.95 | Ĩ | č |
| | ATOM | 453 | Õ | MET I | 66 | 41.389 | 30.829 | -0.688 | 1.00 41.50 | I | 0 |
| | MOTA | 454 | N | LEU I | 67 | 43.485 | 30.009 | -0.723 | 1.00 42.00 | I | N |
| | MOTA | 455 | CA | LEU I | 67 | 43.402 | 29.630 28.838 | 0.683 1.046 | 1.00 42.22 1.00 42.57 | I | C |
| 45 | ATOM ATOM | 456 457 | CB CG | LEU I LEU I | 67 67 | 44.658 44.687 | 27.464 | 0.376 | 1.00 44.35 | Ī | Č |
| | ATOM | 458 | | L LEU I | | 46.052 | 26.785 | 0.490 | 1.00 41.18 | I | C |
| | ATOM | 459 | CD2 | LEU I | 67 | 43.670 | 26.491 | 0.974 | 1.00 42.25 | Ī | C |
| | ATOM | 460 | C | LEU I | 67 | 43.271 | 30.860 | 1.583 | 1.00 41.42 | I | C |
| 50 | ATOM | 461 | O | LEU I SER I | 67 68 | 42.550 44.034 | 30.875 31.912 | 2.572 1.231 | 1.00 39.85 1.00 42.67 | Ï | N O |
| | ATOM ATOM | 462 463 | N CA | SER I | 68 | 43.913 | 33.155 | 1.981 | 1.00 43.98 | Ī | Ĉ |
| | ATOM | 464 | CB | SER I | 68 | 44.801 | 34.206 | 1.314 | 1.00 43.69 | I | С |
| | MOTA | 465 | OG | SER I | 68 | 46.159 | 33.765 | 1.351 | 1.00 46.45 | I | 0 |
| 55 | ATOM | 466 | C | SER I | 68 | 42.460 | 33.632 | 2.008 | 1.00 44.59 1.00 44.55 | I | C |
| | ATOM ATOM | 467 468 | N | SER I GLY I | 68 69 | 41.994 41.747 | 34.271 33.322 | 0.909 | 1.00 45.22 | Ī | N |
| | ATOM | 469 | CA | GLY I | 69 | 40.335 | 33.675 | 0.838 | 1.00 46.25 | I | С |
| | ATOM | 470 | C | GLY I | 69 | 39.526 | 32.989 | 1.942 | 1.00 48.08 | I | C |
| 60 | MOTA | 471 | 0 | GLY I | 69 | 38.600 | 33.548 | 2.515 | 1.00 48.24 | Ī | 0 |
| | ATOM | 472 | N | PHE I | 70 70 | 39.880 | | 2.206 3.249 | 1.00 48.01 1.00 48.55 | I | C N |
| | ATOM | 473 474 | CA CB | PHE I PHE I | 70 70 | 39.178 39.423 | 29.481 | 3.249 | 1.00 49.37 | Ī | C |
| | ATOM ATOM | 475 | CG | | 70 | 38.521 | 28.958 | 1.939 | 1.00 49.79 | I | C |
| 65 | ATOM | 476 | CD: | 1 PHE I | 70 | 39.043 | 28.718 | 0.674 | 1.00 47.81 | I | C |
| | MOTA | 477 | | 2 PHE I | | 37.236 | | 2.253 | 1.00 50.11 | I | G G |
| | MOTA | 478 | | 1 PHE I | | 38.286 36.483 | | -0.269 1.302 | 1.00 47.12 1.00 49.17 | I | C |
| | MOTA MOTA | 479 480 | CE: | | | 37.006 | | 0.041 | 1.00 47.05 | Ī | Č |
| | 222021 | 200 | | | · - | | _ | | | | |

| | 3 5035 | 401 A 1011 | | 39.674 | 31.371 | 4.644 | 1.00 49.59 | I | С |
|------------|--------------|----------------------------|--------------------|------------------|------------------|--------------------|--------------------------|--------|--------------|
| | ATOM ATOM | 481 C PHE 482 O PHE | 1 70 I 70 | 38.995 | 31.218 | 5.651 | 1.00 49.43 | I | 0 |
| • | MOTA | 483 N CYS | I 71 | 40.929 41.534 | 31.858 32.251 | 4.679 5.952 | 1.00 50.98 1.00 51.34 | I I | N C |
| 5 | MOTA MOTA | 484 CA CYS 485 C CYS | I 71 I 71 | 42.194 | 33.617 | 5.844 | 1.00 49.66 | I | С |
| 5 | ATOM | 486 O CYS | I 71 | 43.418 | 33.763 | 5.815 | 1.00 48.07 | I | 0 C |
| | ATOM | 487 CB CYS 488 SG CYS | I 71 I 71 | 42.572 43.274 | 31.188 31.439 | 6.320 7.967 | 1.00 52.25 1.00 56.38 | Ī | s |
| | ATOM ATOM | 488 SG CYS 489 N PRO | | 41.359 | 34.671 | 5.747 | 1.00 49.56 | I | N |
| 10 | ATOM | 490 CD PRO | I 72 | 39.902 | 34.657 | 5.899 | 1.00 48.36 1.00 49.81 | I | C |
| | ATOM | 491 CA PRO 492 CB PRO | | 41.820 40.606 | 36.017 36.853 | 5.495 5.112 | 1.00 49.81 | I | č |
| | ATOM ATOM | 492 CB PRO 493 CG PRO | | 39.372 | 36.152 | 5.670 | 1.00 48.32 | I | C |
| | MOTA | 494 C PRO | I 72 | 42.483 | 36.612 | 6.738 | 1.00 50.31 1.00 49.60 | I I | C O |
| 15 | MOTA | 495 O PRO 496 N HIS | | 43.489 41.834 | 37.301 36.347 | 6.685 7.885 | 1.00 49.60 | Ï | N |
| | ATOM ATOM | 496 N HIS 497 CA HIS | | 42.366 | 36.834 | 9.148 | 1.00 54.75 | I | C |
| | MOTA | 498 CB HIS | I 73 | 41.189 | 37.292 | 10.003 | 1.00 53.22 1.00 51.21 | I I | C |
| | MOTA | 499 CG HIS 500 CD2 HIS | | 40.877 40.029 | 38.728 39.238 | 9.705 8.718 | 1.00 51.21 1.00 49.78 | I | č |
| 20 | ATOM ATOM | 500 CD2 HIS 501 ND1 HIS | | 41.443 | 39.765 | 10.369 | 1.00 50.07 | I | N |
| | ATOM | 502 CE1 HIS | I 73 | 40.952 | 40.876 | 9.787 8.796 | 1.00 52.20 1.00 50.88 | I | C N |
| | MOTA MOTA | 503 NE2 HIS 504 C HIS | | 40.103 43.100 | 40.590 35.735 | 9.890 | 1.00 57.36 | Ī | Ĉ |
| 25 | ATOM | 505 O HIS | | 42.525 | 34.738 | 10.310 | 1.00 56.89 | I | O |
| | MOTA | 506 N LYS | | 44.419 45.102 | 35.908 34.981 | 10.022 10.900 | 1.00 62.03 1.00 66.84 | I | C N |
| | ATOM ATOM | 507 CA LYS 508 CB LYS | | 46.439 | 35.615 | 11.316 | 1.00 66.79 | I | C |
| | MOTA | 509 CG LYS | 5 I 74 | 47.278 | 34.687 | 12.199 | 1.00 67.62 | I I | C |
| 30 | ATOM | 510 CD LYS | | 48.761 49.439 | 35.059 34.791 | 12.195 13.542 | 1.00 67.42 1.00 67.41 | · I | Ċ |
| | MOTA MOTA | 511 CE LYS 512 NZ LYS | | 49.380 | 35.994 | 14.372 | 1.00 66.83 | I | N |
| | ATOM | 513 C LYS | S I 74 | 44.235 | 34.707 | 12.135 | 1.00 70.71 1.00 72.13 | I I | C |
| 0.5 | ATOM | 514 O LYS 515 N VAI | | 44.166 43.487 | 35.504 33.581 | 13.065 12.071 | 1.00 72.13 1.00 76.53 | Ī | И |
| 35 | MOTA MOTA | 515 N VAI 516 CA VAI | | 42.976 | 32.997 | 13.308 | 1.00 80.60 | I | C |
| | ATOM | 517 CB VAI | L 75 | 41.591 | 32.408 | 13.145 | 1.00 80.99 1.00 80.41 | I | C |
| | ATOM | 518 CG1 VAI 519 CG2 VAI | | 41.658 41.258 | 31.357 31.684 | $12.040 \\ 14.447$ | 1.00 80.41 | Ī | Č |
| 40 | ATOM ATOM | | . I 75 | 43.835 | 31.838 | 13.734 | 1.00 83.10 | Ī | C |
| | ATOM | | L T 75 | 43.359 45.127 | 30.786 31.973 | 14.129 13.523 | 1.00 84.01 1.00 86.18 | I | O N |
| | ATOM ATOM | | RI 76 RI 76 | 45.963 | 31.363 | 14.531 | 1.00 88.83 | I | C |
| | MOTA | 524 CB SE | R I 76 | 47.383 | 31.508 | 13.984 | 1.00 89.61 | I | C |
| 45 | MOTA | | RI 76 RI 76 | 47.404 45.692 | 30.931 32.232 | 12.653 15.775 | 1.00 89.51 1.00 90.59 | I | č |
| | ATOM ATOM | | R I 76 R I 76 | 45.810 | 33.452 | 15.712 | 1.00 91.56 | I | 0 |
| | MOTA | 528 N AL | A I 77 | 45.289 | 31.650 | 16.940 17.557 | 1.00 92.05 1.00 92.64 | I | N C |
| 50 | MOTA MOTA | | A I 77 A I 77 | 45.874 45.180 | 30.456 30.233 | 18.903 | 1.00 92.84 | I | C |
| 50 | ATOM | | A I 77 | 45.853 | 29.186 | 16.729 | 1.00 92.83 | Ī | C |
| | MOTA | | A I 77 | 44.830 47.061 | 28.560 28.804 | 16.481 16.299 | 1.00 92.95 1.00 93.00 | I I | N O |
| | MOTA MOTA | | Y I 78 Y I 78 | 47.152 | 27.662 | 15.397 | 1.00 92.73 | I | C |
| 55 | MOTA | 535 C GL | Y I 78 | 48.525 | 27.008 | 15.458 | 1.00 92.58 | I | O C |
| | MOTA | | YI 78 AI 86 | 48.765 52.371 | 26.088 15.408 | 16.231 13.593 | 1.00 93.01 1.00 92.36 | I | N |
| | MOTA MOTA | | A I 86 | 53.584 | 14.621 | 13.409 | 1.00 91.82 | I | C |
| | MOTA | 539 CB AL | A I 86 | 53.416 | 13.774 | 12.147 | 1.00 91.57 1.00 90.72 | I | C |
| 60 | MOTA | | A I 86 A I 86 | 54.820 55.786 | 15.513 15.407 | 13.278 14.021 | 1.00 90.72 | Ī | Õ |
| | ATOM ATOM | | P I 87 | 54.779 | 16.393 | 12.260 | 1.00 89.29 | I | \mathbf{N} |
| | MOTA | 543 CA AS | P I 87 | 55.907 | 17.291 | 12.040 | 1.00 86.83 1.00 87.75 | I | C |
| 6 5 | MOTA | | P I 87 P I 87 | 56.616 56.638 | | 13.377 13.702 | 1.00 87.75 | Ī | C |
| 65 | MOTA ATOM | 546 OD1 AS | | 55.666 | 19.464 | 14.292 | 1.00 89.77 | I | 0 |
| | MOTA | 547 OD2 AS | P I 87 | 57.616 | | 13.367 11.014 | 1.00 88.95 1.00 84.28 | I I | C O |
| | ATOM | | SP I 87 SP I 87 | 56.888 58.074 | | 11.014 | | Ī | ŏ |
| | MOTA | Jaj U As | 0, | 106 | | | | | |

| | ATOM | _ | 8 | 56.342 | 16.382 | 9.831 | 1.00 80.90 | Ĭ | N |
|----|--------------|--|----------|------------------|--------------------|------------------|--------------------------|--------|--------|
| | MOTA | | 8 | 57.188 | 15.835 | 8.777 8.405 | 1.00 77.36 1.00 77.25 | I | C |
| | ATOM | _ | 8 | 56.652 | 14.452 | 8.405 7.753 | 1.00 77.25 | I | C O |
| | MOTA | 333 | 88 | 55.390 | 14.602 | 9.668 | 1.00 77.90 | I | Ċ |
| 5 | ATOM | | 88 | 56.458 | 13.608 16.739 | 7.543 | 1.00 77.01 | Ī | Č |
| | MOTA | _ | 88 88 | 57.202 56.322 | 17.561 | 7.324 | 1.00 75.04 | Ī | ŏ |
| | MOTA | | 39 | 58.272 | 16.591 | 6.740 | 1.00 72.57 | Ĩ | N |
| | MOTA | | 39 | 58.389 | 17.409 | 5.540 | 1.00 70.36 | I | C |
| 10 | MOTA MOTA | | 39 | 59.768 | 18.070 | 5.545 | 1.00 71.28 | I | C |
| 10 | ATOM | | 39 | 59.804 | 19.332 | 6.410 | 1.00 72.04 | I | C |
| | ATOM | | 39 | 60.757 | 20.391 | 5.853 | 1.00 72.01 | I | С |
| | ATOM | | 39 | 60.340 | 21.815 | 6.235 | 1.00 72.21 | I | C |
| | ATOM | | 39 | 61.031 | 22.776 | 5.378 | 1.00 73.09 | I | N |
| 15 | ATOM | | 39 | 58.214 | 16.576 | 4.268 | 1.00 68.20 | I | C |
| | ATOM | | 39 | 59.084 | 15.823 | 3.853 | 1.00 69.41 | I | 0 |
| | ATOM | 300 | 90 | 57.017 | 16.705 | 3.666 | 1.00 63.98 | Ī | N |
| | MOTA | | 90 | 56.741 | 15.960 | 2.443 | 1.00 61.10 | I | C |
| | MOTA | | 90 | 55.316 | 15.412 | 2.531 | 1.00 61.02 | I I | C |
| 20 | ATOM | | 90 | 55.218 | 14.395 | 3.683 | 1.00 60.62 1.00 60.18 | I | C |
| | ATOM | | 90 | 54.332 | $16.548 \\ 16.049$ | $2.824 \\ 2.958$ | 1.00 58.72 | I | Ċ |
| | ATOM | - | 90 90 | 52.892 56.883 | 16.844 | 1.202 | 1.00 59.31 | Ī | č |
| 4 | MOTA | J | 90 | 56.947 | 18.064 | 1.280 | 1.00 60.19 | Ī | ŏ |
| 05 | MOTA | • | 91 | 56.980 | 16.263 | -0.006 | 1.00 57.27 | Ī | N |
| 25 | ATOM ATOM | | 91 | 57.016 | 17.108 | -1.181 | 1.00 56.01 | I | C |
| | ATOM | - | 91 | 57.280 | 16.218 | -2.392 | 1.00 55.94 | I | С |
| | ATOM | | 91 | 58.646 | 15.539 | -2.323 | 1.00 59.79 | I | C |
| | ATOM | | 91 | 58.892 | 14.787 | -3.605 | 1.00 61.27 | I | С |
| 30 | MOTA | | 91 | 60.027 | 14.397 | -3.857 | 1.00 64.11 | I | 0 |
| | MOTA | 580 OE2 GLU I | 91 | 57.935 | 14.589 | -4.343 | 1.00 62.33 | Ξ | 0 |
| | MOTA | 581 C GLU I | 91 | 55.712 | 17.891 | -1.355 | 1.00 54.80 | I | C |
| | MOTA | | 91 | 54.647 | 17.524 | -0.873 | 1.00 55.53 | I | O |
| | MOTA | | 92 | 55.749 | 19.000 | -2.106 | 1.00 53.36 | I | N C |
| 35 | MOTA | | 92 | 54.578 | 19.821 | -2.225 | 1.00 52.86 | I | C |
| | MOTA | | 92 | 54.974 | 21.122 | -2.945 -3.400 | 1.00 53.89 1.00 54.86 | Ī | Ċ |
| | MOTA | | 92 | 53.780 55.646 | 21.945 21.999 | -1.985 | 1.00 53.89 | Ī | č |
| | MOTA | - - · · · · · · · · · · · · · · · · · · | 92 | 53.570 | 19.088 | -3.112 | 1.00 52.07 | Ī | Č |
| 40 | ATOM | | 92 92 | 52.365 | 19.039 | -2.775 | 1.00 49.54 | Ī | ŏ |
| 40 | MOTA | | 93 | 54.048 | 18.417 | -4.204 | 1.00 50.82 | I | N |
| | ATOM ATOM | | 93 | 53.158 | 17.505 | -4.939 | 1.00 51.29 | I | С |
| | ATOM | | 93 | 53.937 | 16.578 | -5.759 | 1.00 51.50 | I | C |
| | ATOM | | 93 | 52.322 | 16.603 | -4.072 | 1.00 51.78 | I | C |
| 45 | ATOM | | 93 | 51.159 | 16.417 | -4.285 | 1.00 52.02 | I | 0 |
| | ATOM | 595 N GLN I | 94 | 52.948 | 15.934 | -3.132 | 1.00 51.82 | I | N |
| | MOTA | 596 CA GLN I | 94 | 52.222 | 15.013 | -2.307 | 1.00 51.43 | I | C |
| | MOTA | 597 CB GLN I | 94 | 53.244 | 14.218 | -1.468 | 1.00 51.33 | Ĭ | C |
| | ATOM | | 94 | 52.539 | 13.173 | -0.468 | 1.00 51.17 1.00 53.13 | I | C |
| 50 | ATOM | | 94 | 52.073 | 11.932 11.461 | -1.233 -1.968 | 1.00 53.13 | Ï | Ö |
| | ATOM | 600 OE1 GLN I | 94 | 52.802 | 11.506 | -1.078 | 1.00 52.92 | Ī | N |
| | ATOM | 601 NE2 GLN I | 94 94 | 50.805 51.354 | 15.741 | -1.330 | 1.00 52.52 | Ī | Ĉ |
| | MOTA | 602 C GLN I 603 O GLN I | 94 | 50.272 | 15.741 | -0.945 | 1.00 51.69 | Ī | Ö |
| 55 | MOTA MOTA | 603 O GLN I 604 N PHE I | 95 | 51.805 | 16.928 | -0.896 | 1.00 48.96 | I | N |
| 33 | ATOM | 605 CA PHE I | 95 | 50.927 | 17.774 | 0.055 | 1.00 46.81 | I | С |
| | ATOM | 606 CB PHE I | 95 | 51.688 | 19.007 | 0.444 | 1.00 44.76 | I | C |
| | ATOM | 607 CG PHE I | 95 | 50.936 | 19.912 | 1.508 | 1.00 45.45 | I | C |
| | MOTA | 608 CD1 PHE I | 95 | 51.118 | 19.792 | 2.777 | 1.00 45.87 | I | С |
| 60 | MOTA | 609 CD2 PHE I | 95 | 49.931 | 20.752 | 1.114 | 1.00 45.94 | I | C |
| | MOTA | 610 CE1 PHE I | 95 | 50.448 | 20.560 | 3.810 | 1.00 45.08 | I | C |
| | ATOM | 611 CE2 PHE I | 95 | 49.271 | 21.524 | 2.109 | 1.00 45.21 | I | C |
| | MOTA | 612 CZ PHE I | 95 | 49.544 | 21.461 | 3.476 | 1.00 44.16 | I | C |
| | MOTA | 613 C PHE I | 95 | 49.687 | 18.134 | -0.632 | 1.00 45.91 1.00 45.21 | I | C |
| 65 | ATOM | 614 O PHE I | 95 | 48.534 | | -0.083 -1.894 | 1.00 45.21 | I | И |
| | ATOM | 615 N VAL I | 96 | 49.843 | 18.547 | -1.894 -2.577 | 1.00 45.24 | I | C |
| | MOTA | 616 CA VAL I | 96 96 | 48.730 49.099 | | -3.820 | 1.00 45.79 | Ī | Č |
| | MOTA | 617 CB VAL I | 96 96 | 47.855 | | -4.467 | 1.00 47.08 | Ī | č |
| | MOTA | 618 CG1 VAL I | 96 | 47.000 | 24.213 | z. ±0/ | 1.00 17.00 | | _ |

| | ATOM | 619 | CG2 VAL I | 96 | 49.696 | 21.210 | -3.547 | 1.00 44.28 | I | С |
|-----------|-----------------|-----|------------|-----|--------|--------|--------|------------|----|----------------|
| | | | | | | | | 1.00 47.34 | Ī | |
| | ATOM | 620 | C VAL I | 96 | 47.825 | 17.939 | -2.988 | | | C |
| | MOTA | 621 | O VAL I | 96 | 46.517 | 18.044 | -3.077 | 1.00 47.21 | I | 0 |
| | MOTA | 622 | N LYS I | 97 | 48.449 | 16.863 | -3.353 | 1.00 49.09 | I | N |
| 5 | ATOM | 623 | CA LYS I | 97 | 47.574 | 15.679 | -3.793 | 1.00 51.55 | Ī | C |
| 5 | | | | | | | | | | |
| | MOTA | 624 | CB LYS I | 97 | 48.493 | 14.584 | -4.189 | 1.00 54.17 | I | С |
| | MOTA | 625 | CG LYS I | 97 | 47.946 | 13.341 | -4.887 | 1.00 60.40 | I. | С |
| | ATOM | 626 | CD LYS I | 97 | 49.050 | 12.597 | -6.011 | 1.00 62.67 | I | Č |
| | | | | | | | | | | ~ |
| | MOTA | 627 | CE LYS I | 97 | 49.068 | 13.410 | -7.468 | 1.00 66.05 | I | C |
| 10 | ATOM | 628 | NZ LYS I | 97 | 50.343 | 13.646 | -8.370 | 1.00 66.57 | I | N |
| | ATOM | 629 | C LYS I | 97 | 46.717 | 15.254 | -2.591 | 1.00 51.16 | I | C |
| | | | | | | | | | | |
| | \mathbf{MOTA} | 630 | O LYS I | 97 | 45.447 | 15.000 | -2.673 | 1.00 50.76 | I | О |
| | MOTA | 631 | N ASP I | 98 | 47.321 | 15.203 | -1.392 | 1.00 52.09 | I | N |
| | ATOM | 632 | CA ASP I | 98 | 46.501 | 14.772 | -0.216 | 1.00 52.20 | I | C |
| | | | | | | | | | | |
| 15 | ATOM | 633 | CB ASP I | 98 | 47.333 | 14.613 | 1.015 | 1.00 54.80 | I | C |
| | ATOM | 634 | CG ASP I | 98 | 48.374 | 13.440 | 0.980 | 1.00 59.19 | I | C |
| | ATOM | 635 | OD1 ASP I | 98 | 49.308 | 13.489 | 1.921 | 1.00 61.38 | I | 0 |
| | | | | | | | | | | |
| | MOTA | 636 | OD2 ASP I | 98 | 48.382 | 12.502 | 0.119 | 1.00 61.58 | Ι | 0 |
| | MOTA | 637 | C ASP I | 98 | 45.449 | 15.883 | 0.089 | 1.00 51.39 | I | C |
| 20 | ATOM | 638 | O ASP I | 98 | 44.352 | 15.575 | 0.548 | 1.00 51.71 | I | 0 |
| 20 | | | | | | | | | | |
| | ATOM | 639 | N LEU I | 99 | 45.774 | 17.198 | -0.106 | 1.00 47.74 | I | N |
| | ATOM | 640 | CA LEU I | 99 | 44.840 | 18.251 | 0.339 | 1.00 47.45 | I | C |
| | ATOM | 641 | CB LEU I | 99 | 45.443 | 19.597 | 0.023 | 1.00 45.49 | I | C |
| | | | | | | | | | | ~ |
| | ATOM | 642 | CG LEU I | 99 | 44.829 | 20.833 | 0.627 | 1.00 44.89 | I | C |
| 25 | MOTA | 643 | CD1 LEU I | 99 | 45.245 | 22.154 | -0.015 | 1.00 43.60 | I | C |
| | MOTA | 644 | CD2 LEU I | 99 | 43.586 | 20.934 | 1.092 | 1.00 43.98 | I | C |
| | | | | | | | | | | Č |
| | MOTA | 645 | C LEU I | 99 | 43.611 | 18.034 | -0.533 | 1.00 46.93 | I | |
| | ATOM | 646 | O LEU I | 99 | 42.468 | 18.230 | -0.102 | 1.00 47.46 | I | 0 |
| | ATOM | 647 | N LEU I | 100 | 43.851 | 17.760 | -1.794 | 1.00 45.76 | I | N |
| 20 | | | | | 42.817 | 17.754 | -2.807 | | Ī | Ĉ |
| 30 | MOTA | 648 | CA LEU I | | | | | 1.00 44.53 | | |
| | ATOM | 649 | CB LEU I | | 43.591 | 17.644 | -4.248 | 1.00 43.55 | I | C |
| | MOTA | 650 | CG LEU I | 100 | 42.669 | 17.411 | -5.353 | 1.00 43.64 | I | C |
| | | | CD1 LEU I | | 41.718 | 18.519 | -5.349 | 1.00 42.86 | I | Č |
| | MOTA | 651 | | | | | | | | |
| | MOTA | 652 | CD2 LEU I | 100 | 43.369 | 17.199 | -6.753 | 1.00 40.11 | I | C |
| 35 | ATOM | 653 | C LEU I | 100 | 41.890 | 16.646 | -2.616 | 1.00 44.86 | I | C |
| | ATOM | 654 | O LEU I | | 40.620 | 16.754 | -2.540 | 1.00 45.24 | I | Õ |
| | | | | | | | | | | |
| | ATOM | 655 | N LEU I | 101 | 42.441 | 15.498 | -2.233 | 1.00 45.36 | I | N |
| | MOTA | 656 | CA LEU I | 101 | 41.532 | 14.416 | -1.832 | 1.00 46.01 | Ι | C |
| | | 657 | CB LEU I | | 42.304 | 13.119 | -1.634 | 1.00 45.92 | I | Č |
| | ATOM | | | | | | | | | |
| 40 | MOTA | 658 | CG LEU I | | 42.851 | 12.537 | -2.978 | 1.00 45.91 | I | С |
| | MOTA | 659 | CD1 LEU I | 101 | 43.906 | 11.504 | -2.808 | 1.00 46.51 | I | C |
| | ATOM | 660 | CD2 LEU I | | 41.696 | 11.862 | -3.903 | 1.00 43.07 | I | C |
| | | | | | | | | | | $\tilde{\sim}$ |
| | MOTA | 661 | C LEU I | | 40.596 | 14.747 | -0.682 | 1.00 46.66 | I | C |
| | ATOM | 662 | O LEU I | 101 | 39.288 | 14.481 | -0.628 | 1.00 48.00 | I | 0 |
| 45 | ATOM | 663 | N HIS I | | 41.150 | 15.486 | 0.214 | 1.00 46.69 | I | N |
| -10 | | | | | | | | | Ī | |
| | MOTA | 664 | CA HIS I | | 40.320 | 15.789 | 1.334 | 1.00 48.31 | | C |
| | MOTA | 665 | CB HIS I | 102 | 41.194 | 16.406 | 2.430 | 1.00 51.03 | I | С |
| | ATOM | 666 | CG HIS I | 102 | 40.434 | 16.774 | 3.641 | 1.00 51.82 | I | C |
| | ATOM | 667 | CD2 HIS I | | 40.061 | 17.963 | 4.107 | 1.00 53.23 | I | C |
| 50 | | | | | | | | | | |
| 50 | ATOM | 668 | ND1 HIS I | | 40.122 | 15.873 | 4.610 | 1.00 53.12 | I | N |
| | MOTA | 669 | CE1 HIS I | 102 | 39.380 | 16.456 | 5.518 | 1.00 54.50 | I | C |
| | ATOM | 670 | NE2 HIS I | | 39.373 | 17.741 | 5.260 | 1.00 56.06 | I | N |
| | | | MEE HILD I | 102 | 30.373 | | | | | |
| | MOTA | 671 | C HIS I | | 39.281 | 16.813 | 0.903 | 1.00 48.41 | I | C |
| | ATOM | 672 | O HIS I | 102 | 38.102 | 16.806 | 1.343 | 1.00 46.87 | I | 0 |
| 55 | MOTA | 673 | N LEU I | | 39.724 | 17.763 | 0.094 | 1.00 48.47 | I | N |
| 55 | | | | | | | | | | |
| | \mathbf{MOTA} | 674 | CA LEU I | | 38.678 | 18.709 | -0.307 | 1.00 49.56 | I | C |
| | MOTA | 675 | CB LEU I | 103 | 39.292 | 19.869 | -1.094 | 1.00 48.48 | I | C |
| | ATOM | 676 | CG LEU I | | 40.354 | 20.788 | -0.467 | 1.00 49.09 | Ī | Ċ |
| | | | | | | | | | | ~ |
| | MOTA | 677 | CD1 LEU I | | 41.044 | 21.809 | -1.341 | 1.00 49.00 | I | C |
| 60 | MOTA | 678 | CD2 LEU I | 103 | 39.733 | 21.564 | 0.838 | 1.00 45.10 | I | C |
| | ATOM | 679 | C LEU I | | 37.585 | 18.095 | -1.176 | 1.00 50.10 | I | Ċ |
| | | | | | | | | | | |
| | MOTA | 680 | O LEU I | | 36.461 | 18.432 | -1.074 | 1.00 49.95 | I | 0 |
| | ATOM | 681 | N LYS I | 104 | 37.937 | 17.154 | -2.005 | 1.00 50.85 | I | N |
| | ATOM | 682 | CA LYS I | | 36.867 | 16.490 | -2.802 | 1.00 50.86 | I | C |
| CE | | | | | | | | | | \tilde{a} |
| 65 | MOTA | 683 | CB LYS I | | 37.402 | 15.549 | -3.797 | 1.00 49.12 | I | С |
| | ATOM | 684 | CG LYS I | 104 | 38.306 | 16.284 | -4.777 | 1.00 48.40 | I | С |
| | ATOM | 685 | CD LYS I | 104 | 38.591 | 15.250 | -5.921 | 1.00 47.57 | I | Č |
| | | | | | | | | | | |
| | MOTA | 686 | CE LYS I | | 39.248 | 15.985 | -7.140 | 1.00 48.88 | I | C |
| | MOTA | 687 | NZ LYS I | 104 | 39.306 | 15.204 | -8.323 | 1.00 47.96 | I | N |
| | | | | | | | | | | |

| | ATOM ATOM ATOM | 688 689 690 | C O N | LYS I LYS I LYS I | 104 104 105 | 35.925 34.706 36.454 | 15.737 15.596 15.185 | -1.861 -2.147 -0.819 | 1.00 50.92 1.00 50.71 1.00 52.08 | | C C C N |
|----|------------------------------|--------------------------|-------------------------|----------------------------------|--------------------------|--------------------------------------|--------------------------------------|--------------------------------------|--|---|--------------------------|
| 5 | MOTA MOTA MOTA MOTA | 691 692 693 694 | CA CB CG CD | LYS I | 105 105 105 105 | 35.547 36.263 35.474 36.344 | 14.557 13.771 13.493 13.038 | 0.142 1.148 2.486 3.615 | 1.00 54.25 1.00 56.55 1.00 60.33 1.00 63.22 | - | |
| 10 | ATOM ATOM ATOM | 695 696 697 | CE NZ C | LYS I LYS I LYS I | 105 105 105 | 36.799 37.722 34.658 | 11.582 11.200 15.480 | 3.364 4.601 0.879 | 1.00 66.16 1.00 71.27 1.00 54.66 | - | E C |
| | ATOM ATOM ATOM ATOM | 698 699 700 701 | O N CA CB | LYS I LEU I LEU I | 106 | 33.426 35.161 34.246 35.016 | 15.193 16.673 17.681 18.909 | 0.899 1.347 1.925 2.367 | 1.00 54.59 1.00 55.31 1.00 55.19 1.00 55.63 | : | E C |
| 15 | ATOM ATOM ATOM | 702 703 704 | CG CD1 CD2 | LEU I LEU I | 106 106 | 36.158 36.737 35.581 | 18.689 20.087 18.001 | 3.345 3.680 4.446 | 1.00 56.60 1.00 56.04 1.00 56.80 | - | I C |
| 20 | ATOM ATOM ATOM ATOM | 705 706 707 708 | C N CA | | 106 107 | 33.206 32.049 33.576 32.581 | 18.130 18.328 18.256 18.731 | 0.944 1.266 -0.333 -1.318 | 1.00 55.25 1.00 53.51 1.00 55.92 1.00 56.04 | | I C I O I C |
| 05 | ATOM ATOM ATOM | 709 710 711 | CB CG CD1 | PHE I PHE I | 107 107 | 33.229 32.373 32.040 | 18.776 19.340 20.666 | -2.639 -3.734 -3.816 | 1.00 53.89 1.00 52.39 1.00 52.13 1.00 52.09 | : | |
| 25 | ATOM ATOM ATOM ATOM | 712 713 714 715 | CD2 CE1 CE2 CZ | PHE I PHE I PHE I | 107 107 | 31.786 31.227 30.982 30.726 | 18.487 21.177 18.929 20.235 | -4.567 -4.966 -5.609 -5.871 | 1.00 52.09 1.00 53.21 1.00 52.54 1.00 51.78 | | |
| 30 | ATOM ATOM ATOM | 716 717 718 | О И | PHE I PHE I ARG I | 107 108 | 31.505 30.309 31.891 | 17.720 17.986 16.490 | -1.389 -1.382 -1.534 | 1.00 57.69 1.00 57.18 1.00 60.03 | : | C C O |
| 35 | ATOM ATOM ATOM ATOM | 719 720 721 722 | CA CB CG CD | ARG I ARG I ARG I | 108 | 30.881 31.608 30.754 31.667 | 15.511 14.199 12.873 11.584 | -1.665 -2.008 -2.025 -2.519 | 1.00 63.96 1.00 65.15 1.00 67.16 1.00 68.85 | - | |
| | MOTA MOTA MOTA | 723 724 725 | NE CZ NH1 | ARG I ARG I ARG I | 108 108 108 | 32.695 34.069 34.757 | 11.003 11.182 11.989 | -1.599 -1.590 -2.451 | 1.00 70.00 1.00 70.81 1.00 70.77 | - | E C |
| 40 | ATOM ATOM ATOM ATOM | 726 727 728 729 | NH2 C O N | ARG I | | 34.784 29.994 28.819 30.524 | 10.519 15.439 15.168 15.646 | -0.653 -0.290 -0.358 0.926 | 1.00 70.34 1.00 66.09 1.00 66.77 1.00 68.31 | - | E N E O E N |
| 45 | ATOM ATOM ATOM | 730 731 732 | CA CB CG | GLU I GLU I GLU I | 109 109 109 | 29.675 30.552 31.156 | 15.629 15.413 14.032 | 2.113 3.334 3.348 | 1.00 70.48 1.00 72.41 1.00 74.96 | - | T C |
| | ATOM ATOM ATOM ATOM | 733 734 735 736 | CD OE1 OE2 C | GLU I GLU I GLU I | 109 109 | 32.329 32.637 32.937 28.905 | 13.680 12.428 14.563 16.948 | 4.311 4.269 5.045 2.276 | 1.00 77.15 1.00 77.91 1.00 78.45 1.00 71.26 | - | |
| 50 | ATOM ATOM ATOM | 737 738 739 | O N CA | GLY I GLY I | 109 110 110 | 28.156 29.031 28.285 | 17.047 17.967 19.190 | 3.145 1.442 1.716 | 1.00 72.42 1.00 71.47 1.00 72.78 | - | E C |
| 55 | ATOM ATOM ATOM ATOM | 740 741 742 743 | C O N CA | GLY I GLY I ARG I ARG I | 110 111 | 28.749 27.929 30.065 30.802 | 20.232 20.900 20.280 21.114 | 2.811 3.473 3.036 3.976 | 1.00 73.70 1.00 73.73 1.00 74.76 1.00 75.92 | | E C |
| | ATOM ATOM ATOM | 744 745 746 | CB CG CD | ARG I ARG I ARG I | 111 111 | 31.695 30.977 31.331 | 20.202 18.919 18.500 | 4.816 5.233 6.664 | 1.00 76.34 1.00 77.70 1.00 79.60 | - | |
| 60 | ATOM ATOM ATOM | 747 748 749 | NE CZ NH1 | | 111 111 | 32.505 33.534 33.458 | 17.621 17.966 19.050 | 6.665 7.461 8.214 | 1.00 80.80 1.00 81.19 1.00 80.98 | - | I N I C I N |
| 65 | ATOM ATOM ATOM ATOM | 750 751 752 753 | C O N | ARG I ARG I ARG I PHE I | 111 111 | 34.641 31.650 32.822 30.996 | 17.219 22.165 21.971 23.297 | 7.470 3.253 2.955 2.931 | 1.00 81.56 1.00 76.69 1.00 75.67 1.00 78.04 | - | I N I C I O I N |
| | ATOM ATOM ATOM | 754 755 756 | CA CB CG | PHE I PHE I PHE I | 112 112 | 31.701 30.682 30.167 | 24.365 25.138 24.261 | 2.230 1.392 0.290 | 1.00 79.36 1.00 79.30 1.00 78.67 | 2 | E C |

| | | | | | | | _ | _ |
|---------|------------------|--|------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM | 757 CD1 PHE 1 112 | 30.576 | 24.490 | -1.018 | 1.00 78.26 1.00 78.46 | I I | C C |
| | MOTA | 758 CD2 PHE I 112 | 29.326 | 23.201 23.643 | 0.586 -2.030 | 1.00 78.46 | I | C |
| | MOTA | 759 CE1 PHE I 112 760 CE2 PHE I 112 | 30.147 28.901 | 22.357 | -0.435 | 1.00 79.06 | Ī | Č |
| | MOTA | 760 CE2 PHE I 112 761 CZ PHE I 112 | 29.311 | 22.571 | -1.744 | 1.00 78.48 | I | С |
| 5 | ATOM ATOM | 762 C PHE I 112 | 32.402 | 25.314 | 3.205 | 1.00 79.89 | I | C |
| | ATOM | 763 O PHE I 112 | 32.665 | 26.470 | 2.905 | 1.00 79.55 | I | 0 |
| | ATOM | 764 OXT PHE I 112 | 32.729 | 24.958 | 4.329 | 1.00 81.92 1.00109.80 | I R | 0 |
| | MOTA | 765 CB PRO R 33 | 77.296 | 6.508 7.071 | 12.091 13.466 | 1.00109.72 | R | Č |
| 10 | MOTA | 766 CG PRO R 33 767 C PRO R 33 | 77.634 75.600 | 7.448 | 10.489 | 1.00109.45 | R | č |
| | ATOM | | 74.661 | 8.222 | 10.616 | 1.00109.75 | R | 0 |
| | ATOM ATOM | 768 O PROR 33 769 N PROR 33 | .76.843 | 8.883 | 12.021 | 1.00109.73 | R | N |
| | ATOM | 770 CD PRO R 33 | 76.862 | 8.467 | 13.415 | 1.00110.08 | R | C |
| 15 | ATOM | 771 CA PRO R 33 | 76.935 | 7.688 | 11.188 | 1.00109.68 | R R | C N |
| | MOTA | 772 N PROR 34 | 75.508 | 6.367 | 9.699 9.479 | 1.00108.90 1.00108.56 | R | C |
| | MOTA | 773 CD PRO R 34 | 76.393 74.287 | 5.227 6.191 | 8.965 | 1.00108.17 | R | Č |
| | ATOM | 774 CA PRO R 34 775 CB PRO R 34 | 74.529 | 5.074 | 7.955 | 1.00108.27 | R | С |
| 00 | ATOM ATOM | 775 CB PRO R 34 776 CG PRO R 34 | 75.702 | 4.241 | 8.433 | 1.00108.37 | R | C |
| 20 | MOTA | 777 C PRO R 34 | 73.222 | 5.747 | 9.912 | 1.00107.50 | R | C |
| | MOTA | 778 O PROR 34 | 73.082 | 6.166 | 11.048 | 1.00107.84 | R R | N O |
| | MOTA | 779 N VAL R 35 | 72.413 | 4.851 | 9.403 | 1.00106.22 1.00105.21 | R | G |
| | MOTA | 780 CA VAL R 35 | 71.466 | $4.319 \\ 4.467$ | 10.308 9.738 | 1.00105.21 | R | č |
| 25 | MOTA | 781 CB VAL R 35 782 CG1 VAL R 35 | 70.119 | 5.236 | 8.419 | 1.00104.78 | R | С |
| | ATOM ATOM | 782 CG1 VAL R 35 783 CG2 VAL R 35 | 69.432 | 3.095 | 9.498 | 1.00105.97 | R | C |
| | ATOM | 784 C VAL R 35 | 71.756 | 2.861 | 10.581 | 1.00104.36 | R | C |
| | ATOM | 785 O VAL R 35 | 72.155 | 2.089 | 9.684 | 1.00104.20 | R | O N |
| 30 | ATOM | 786 N THR R 36 | 71.618 | 2.545 | 11.858 12.159 | 1.00103.37 1.00101.83 | R R | C |
| | MOTA | 787 CA THR R 36 | 71.682 72.110 | 1.191 0.938 | 13.626 | 1.00101.03 | R | č |
| | ATOM | 788 CB THR R 36 789 OG1 THR R 36 | 73.534 | 0.821 | 13.586 | 1.00102.34 | R | 0 |
| | ATOM ATOM | 789 OG1 THR R 36 790 CG2 THR R 36 | 71.552 | -0.439 | 14.041 | 1.00101.87 | R | С |
| 35 | ATOM | 791 C THR R 36 | 70.527 | 0.342 | 11.738 | 1.00100.49 | R | C |
| 00 | MOTA | 792 O THR R 36 | 69.352 | 0.681 | 11.806 | 1.00100.30 | R R | N O |
| | MOTA | 793 N ASN R 37 | 71.068 | -0.838 | 11.402 | 1.00 98.77 1.00 97.02 | R | C |
| | MOTA | 794 CA ASN R 37 | 70.689 69.950 | -1.982 -3.094 | 10.491 11.245 | 1.00 97.91 | R | č |
| | MOTA | 795 CB ASN R 37 796 CG ASN R 37 | 69.677 | -2.566 | 12.592 | 1.00 98.59 | R | C |
| 40 | MOTA MOTA | 796 CG ASN R 37 797 OD1 ASN R 37 | 69.061 | -1.530 | 12.693 | 1.00 99.04 | R | 0 |
| | MOTA | 798 ND2 ASN R 37 | 70.269 | -3.216 | 13.594 | 1.00 98.75 | R | И |
| | ATOM | 799 C ASN R 37 | 70.302 | -1.704 | 9.042 | 1.00 95.59 | R R | O |
| | MOTA | 800 O ASN R 37 | 71.128 | -1.673 | 8.134 8.942 | 1.00 95.97 1.00 92.71 | R | N |
| 45 | MOTA | 801 N LEUR 38 802 CA LEUR 38 | 68.988 68.261 | -1.564 -1.183 | 7.691 | 1.00 89.88 | R | Ĉ |
| | MOTA | 802 CA LEUR 38 803 CB LEUR 38 | 68.999 | | 6.719 | 1.00 89.18 | R | С |
| | ATOM ATOM | 804 CG LEU R 38 | 67.999 | | 5.670 | 1.00 88.71 | R | C |
| | ATOM | 805 CD1 LEU R 38 | 67.016 | 1.337 | 6.281 | 1.00 87.75 | R | C |
| 50 | ATOM | 806 CD2 LEU R 38 | 68.648 | | 4.469 | 1.00 88.12 1.00 88.31 | R R | C |
| | MOTA | 807 C LEUR 38 | 67.588 68.101 | | 6.945 5.943 | 1.00 88.23 | R | ŏ |
| | ATOM | 808 O LEUR 38 809 N SERR 39 | 66.424 | | 7.462 | 1.00 86.43 | R | N |
| | MOTA MOTA | 809 N SER R 39 810 CA SER R 39 | 65.722 | | 6.933 | 1.00 85.04 | Ŕ | C |
| 55 | MOTA | 811 CB SER R 39 | 65.446 | | 8.104 | 1.00 84.80 | R | C |
| 00 | MOTA | 812 OG SER R 39 | 64.399 | | 8.906 | 1.00 84.68 | R | 0 |
| | MOTA | 813 C SER R 39 | 64.391 | | 6.246 6.301 | 1.00 83.83 1.00 83.04 | R R | Ö |
| | ATOM | 814 O SER R 39 | 63.917 | | | | R | N |
| | MOTA | 815 N VAL R 40 816 CA VAL R 40 | 63.820 62.586 | | | | R | C |
| 60 | MOTA | 816 CA VAL R 40 817 CB VAL R 40 | 62.951 | | 3.340 | 1.00 81.55 | R | С |
| | MOTA MOTA | 818 CG1 VAL R 40 | 63.536 | | 2.743 | 1.00 81.22 | R | C |
| | MOTA | 819 CG2 VAL R 40 | 61.713 | 3 -3.716 | 2.557 | | R | C |
| | MOTA | 820 C VAL R 40 | 61.596 | | | | R R | C |
| 65 | MOTA | 821 O VAL R 40 | 61.958 | | | | R | N |
| | ATOM | 822 N SER R 41 823 CA SER R 41 | 60.299 59.25 | | | | R | С |
| | ATOM | 823 CA SER R 41 824 CB SER R 41 | 58.69 | | | 1.00 79.25 | R | С |
| | $f MOTA \\ MOTA$ | 825 OG SER R 41 | 57.87 | | | | R | 0 |
| | AIOM | | 100 | | | | | |

| | ATOM ATOM ATOM | 826 827 828 | C SER R O SER R N VAL R | 41 41 42 | 58.139 58.133 57.188 | -5.936 -4.987 -6.889 | 4.032 3.260 4.011 | 1.00 78.20 1.00 78.12 1.00 77.02 | R R R | C O N |
|----|------------------------------|--------------------------|--|----------------------|--------------------------------------|--------------------------------------|--------------------------------------|--|--------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM | 829 830 831 832 | CA VAL R CB VAL R CG1 VAL R CG2 VAL R | 42 42 42 42 | 56.044 56.345 55.040 57.239 | -6.727 -7.421 -7.685 -6.540 | 3.122 1.793 1.042 0.940 | 1.00 75.75 1.00 75.63 1.00 74.23 1.00 75.00 | R . R R R | C C C |
| 10 | ATOM ATOM ATOM | 833 834 835 | C VAL R O VAL R N GLU R | 42 42 43 | 54.757 54.456 54.009 | -7.294 -8.476 -6.404 | 3.725 3.634 4.401 | 1.00 75.25 1.00 76.26 1.00 74.69 | R R R | C N |
| | ATOM ATOM ATOM ATOM | 836 837 838 839 | CA GLU R CB GLU R CG GLU R CD GLU R | 43 43 43 43 | 52.690 52.364 53.535 53.105 | -6.791 -5.955 -5.884 -5.130 | 4.879 6.118 7.101 8.339 | 1.00 74.33 1.00 74.91 1.00 76.67 1.00 78.12 | R R R R | 2000 |
| 15 | ATOM ATOM ATOM | 840 841 842 | OE1 GLU R OE2 GLU R C GLU R | 43 43 43 | 52.040 53.849 51.628 | -4.530 -5.147 -6.569 | 8.320 9.319 3.802 | 1.00 78.66 1.00 78.91 1.00 73.28 | R R R | 0 0 |
| 20 | ATOM ATOM ATOM ATOM | 843 844 845 846 | O GLUR N ASNR CA ASNR CB ASNR | 43 44 44 44 | 51.886 50.404 49.329 49.105 | -6.038 -7.036 -6.870 -5.371 | 2.730 4.102 3.133 2.930 | 1.00 72.01 1.00 73.87 1.00 73.91 1.00 74.10 | R R R R | 0 N C C |
| 05 | ATOM ATOM ATOM | 847 848 849 850 | CG ASN R OD1 ASN R ND2 ASN R C ASN R | 44 44 44 44 | 48.598 48.998 47.676 49.681 | -4.762 -3.674 -5.493 -7.528 | 4.211 4.615 4.861 1.798 | 1.00 73.66 1.00 73.71 1.00 72.65 1.00 74.25 | R R R | С И С |
| 25 | ATOM ATOM ATOM ATOM | 851 852 853 | C ASN R O ASN R N LEU R CA LEU R | 44 45 45 | 50.000 49.577 49.894 | -7.328 -8.706 -6.724 -7.249 | 1.712 0.725 -0.598 | 1.00 74.23 1.00 74.82 1.00 74.52 1.00 73.93 | R R R | 0 N |
| 30 | ATOM ATOM ATOM ATOM | 854 855 856 857 | CB LEU R CG LEU R CD1 LEU R CD2 LEU R | 45 45 45 45 | 48.630 48.034 46.992 49.086 | -7.177 -8.558 -8.520 -9.581 | -1.455 -1.742 -2.860 -2.172 | 1.00 75.60 1.00 77.31 1.00 76.95 1.00 77.38 | R R R R | 0000 |
| 35 | ATOM ATOM ATOM | 858 859 860 | C LEU R O LEU R N CYS R | 45 45 46 | 51.020 51.867 50.984 | -6.452 -6.982 -5.124 | -1.261 -1.968 -1.041 | 1.00 73.85 1.00 73.55 1.00 73.09 | R R R | И О С |
| | ATOM ATOM ATOM ATOM | 861 862 863 864 | CA CYS R CB CYS R SG CYS R C CYS R | 46 46 46 46 | 52.004 51.354 50.633 52.629 | -4.267 -3.448 -4.496 -3.335 | -1.633 -2.750 -4.034 -0.593 | 1.00 72.73 1.00 73.79 1.00 79.48 1.00 71.57 | R R R R | C S C |
| 40 | ATOM ATOM ATOM | 865 866 867 | O CYS R N THR R CA THR R | 46 47 47 | 53.638 51.964 52.489 | -2.680 -3.262 -2.429 | -0.821 0.575 1.650 | 1.00 71.95 1.00 70.15 1.00 69.21 | R R R | 0 N C |
| 45 | ATOM ATOM ATOM ATOM | 868 869 870 871 | CB THR R OG1 THR R CG2 THR R C THR R | 47 47 47 47 | 51.529 50.203 51.918 53.886 | -2.523 -2.240 -1.501 -2.880 | 2.836 2.387 3.909 2.078 | 1.00 69.25 1.00 69.24 1.00 68.49 1.00 68.94 | R R R R | 0000 |
| | MOTA MOTA MOTA | 872 873 874 | O THR R N VAL R CA VAL R | 47 48 48 | 54.063 54.903 56.280 | -3.827 -2.190 -2.524 | 2.834 1.526 1.874 | 1.00 69.53 1.00 68.05 1.00 68.58 | R R R | О И О |
| 50 | ATOM ATOM ATOM ATOM | 875 876 877 878 | CB VAL R CG1 VAL R CG2 VAL R C VAL R | 48 48 48 48 | 57.128 56.460 58.510 56.831 | -2.444 -1.520 -1.913 -1.570 | 0.603 -0.415 0.930 2.939 | 1.00 67.24 1.00 69.11 1.00 67.36 1.00 68.62 | R R R R | 0 0 0 |
| 55 | MOTA ATOM MOTA | 879 880 881 | O VAL R N ILE R CA ILE R | 48 49 49 | 56.755 57.366 57.817 | -0.354 -2.165 -1.346 | 2.828 4.020 5.141 | 1.00 69.25 1.00 69.02 1.00 68.84 | R R R | O N C |
| 60 | ATOM ATOM ATOM ATOM | 882 883 884 885 | CB ILE R CG2 ILE R CG1 ILE R CD1 ILE R | 49 49 49 49 | 57.145 57.520 55.621 54.895 | -1.876 -0.994 -1.837 -2.073 | 6.407 7.611 6.253 7.578 | 1.00 68.78 1.00 68.35 1.00 68.17 1.00 70.58 | R R R R | 0 0 0 |
| | MOTA MOTA MOTA | 886 887 888 | C ILE R O ILE R N TRP R | 49 49 50 | 59.340 59.988 59.880 | -1.378 -2.402 -0.181 | 5.303 5.128 5.604 | 1.00 68.46 1.00 69.77 1.00 67.57 | R R R | С О И |
| 65 | ATOM ATOM ATOM ATOM | 889 890 891 892 | CA TRP R CB TRP R CG TRP R CD2 TRP R | 50 50 50 50 | 61.301 61.923 62.451 61.786 | -0.080 1.007 0.431 0.431 | 5.915 5.035 3.778 2.493 | 1.00 67.76 1.00 65.27 1.00 63.09 1.00 62.66 | R R R R | 0 0 0 |
| | ATOM MOTA | 893 894 | CE2 TRP R CE3 TRP R | 50 50 | 62.701 60.515 | -0.093 0.815 | 1.546 2.077 | 1.00 62.24 1.00 61.27 | R R | C |

| | ATOM | 895 | CD1 | TRP R | 50 | 6 | 3.743 | -0.102 | 3.562 | 1.00 63.41 | R | C |
|-----|------|-----|---------|-------|----------|------------|--------|--------|--------|--------------------------|--------|---|
| | | 896 | | TRP R | 50 | | 3.958 | -0.433 | 2.260 | 1.00 61.66 | R | N |
| | ATOM | | | | | - | | -0.227 | 0.220 | 1.00 62.59 | R | Ĉ |
| | ATOM | 897 | CZ2 | TRP R | 50 | | 2.320 | | | | R | |
| | ATOM | 898 | | TRP R | 50 | | 0.133 | 0.678 | 0.754 | 1.00 61.70 | | C |
| 5 | MOTA | 899 | | TRP R | 50 | | 1.045 | 0.158 | -0.182 | 1.00 63.14 | R | C |
| | ATOM | 900 | С | TRP R | 50 | | 1.514 | 0.280 | 7.383 | 1.00 69.60 | R | C |
| | MOTA | 901 | 0 | TRP R | 50 | | 50.901 | 1.187 | 7.933 | 1.00 71.18 | R | 0 |
| | ATOM | 902 | N | THR R | 51 | | 52.395 | -0.499 | 8.030 | 1.00 71.70 | R | N |
| | ATOM | 903 | CA | THR R | 51 | ϵ | 52.717 | -0.217 | 9.414 | 1.00 73.55 | R | C |
| 10 | ATOM | 904 | CB | THR R | 51 | 6 | 2.099 | -1.313 | 10.283 | 1.00 72.56 | R | С |
| | ATOM | 905 | OG1 | THR R | 51 | 6 | 52.465 | -2.591 | 9.761 | 1.00 72.81 | R | 0 |
| | ATOM | 906 | CG2 | THR R | 51 | 6 | 50.571 | -1.190 | 10.271 | 1.00 72.22 | R | C |
| | ATOM | 907 | C | THR R | 51 | | 4.221 | -0.181 | 9.612 | 1.00 75.37 | R | С |
| | ATOM | 908 | ŏ | THR R | 51 | | 54.995 | -0.852 | 8.937 | 1.00 75.38 | R | Ō |
| 4 = | | | | TRP R | 52 | | 54.635 | 0.683 | 10.543 | 1.00 77.41 | R | N |
| 15 | ATOM | 909 | N | | 52 | | 6.052 | 0.795 | 10.814 | 1.00 79.26 | R | Ċ |
| | ATOM | 910 | CA | TRP R | | | | 1.724 | 9.758 | 1.00 79.75 | R | Č |
| | ATOM | 911 | CB | TRP R | 52 | | 66.668 | | | | R | Č |
| | ATOM | 912 | CG | TRP R | 52 | | 56.114 | 3.093 | 9.875 | 1.00 80.89 | | |
| | MOTA | 913 | CD2 | TRP R | 52 | | 55.067 | 3.675 | 9.057 | 1.00 81.56 | R | C |
| 20 | MOTA | 914 | CE2 | TRP R | 52 | | 54.989 | 5.051 | 9.392 | 1.00 81.99 | R | C |
| | ATOM | 915 | CE3 | TRP R | 52 | | 54.192 | 3.155 | 8.106 | 1.00 81.29 | R | C |
| | MOTA | 916 | CD1 | TRP R | 52 | (| 56.624 | 4.141 | 10.674 | 1.00 81.45 | R | С |
| | ATOM | 917 | NE1 | TRP R | 52 | (| 56.009 | 5.331 | 10.431 | 1.00 81.21 | R | N |
| | ATOM | 918 | CZ2 | TRP R | 52 | (| 54.052 | 5.864 | 8.772 | 1.00 81.96 | R | С |
| 25 | ATOM | 919 | CZ3 | TRP R | 52 | (| 53.255 | 3.967 | 7.488 | 1.00 81.08 | R | C |
| | MOTA | 920 | CH2 | TRP R | 52 | | 53.183 | 5.329 | 7.828 | 1.00 81.26 | R | C |
| | MOTA | 921 | C | TRP R | 52 | | 56.293 | 1.345 | 12.208 | 1.00 80.42 | R | C |
| | ATOM | 922 | ŏ | TRP R | 52 | | 55.384 | 1.531 | 13.007 | 1.00 79.43 | R | 0 |
| | | 923 | N | ASN R | 53 | | 57.563 | 1.568 | 12.523 | 1.00 82.95 | R | N |
| 00 | ATOM | 924 | | ASN R | 53 | | 57.829 | 2.105 | 13.838 | 1.00 85.26 | R | Ĉ |
| 30 | MOTA | | CA | | | | 68.545 | 1.040 | 14.660 | 1.00 86.57 | R | č |
| | ATOM | 925 | CB | ASN R | 53 | | | 0.038 | 15.127 | 1.00 88.41 | R | Č |
| | MOTA | 926 | CG | ASN R | 53 | | 67.526 | | | | | Ö |
| | MOTA | 927 | | ASN R | 53 | | 66.721 | 0.304 | 16.014 | 1.00 89.46 | R | |
| | ATOM | 928 | . ND2 | | 53 | | 67.493 | -1.103 | 14.423 | 1.00 88.47 | R | N |
| 35 | MOTA | 929 | C | ASN R | 53 | | 68.657 | 3.371 | 13.780 | 1.00 85.99 | R | C |
| | MOTA | 930 | 0 | ASN R | 53 | | 69.353 | 3.661 | 12.814 | 1.00 84.91 | R | 0 |
| | MOTA | 931 | N | PRO R | 54 | 1 | 68.513 | 4.161 | 14.854 | 1.00 87.46 | R | N |
| | ATOM | 932 | CD | PRO R | 54 | | 67.558 | 4.031 | 15.939 | 1.00 87.13 | R | C |
| | ATOM | 933 | CA | PRO R | 54 | | 69.367 | 5.306 | 15.068 | 1.00 88.96 | R | C |
| 40 | ATOM | 934 | CB | PRO R | 54 | | 69.022 | 5.900 | 16.433 | 1.00 88.51 | R | C |
| 1.0 | ATOM | 935 | CG | PRO R | 54 | | 67.670 | 5.336 | 16.857 | 1.00 87.81 | R | С |
| | ATOM | 936 | C | PRO R | 54 | | 70.837 | 4.875 | 15.020 | 1.00 91.16 | R | C |
| | ATOM | 937 | ŏ | PRO R | 54 | | 71.225 | 3.786 | 15.408 | 1.00 91.95 | R | 0 |
| | MOTA | 938 | N | PRO R | 55 | | 71.659 | 5.767 | 14.471 | 1.00 92.77 | R | N |
| 4E | | 939 | CD | PRO R | 55 | | 71.358 | 7.124 | 14.076 | 1.00 92.90 | R | Ċ |
| 45 | ATOM | | | | 55 55 | | 73.060 | 5.474 | 14.196 | 1.00 94.38 | R | Č |
| | ATOM | 940 | CA | PRO R | | | | | 13.888 | 1.00 93.93 | R | Č |
| | MOTA | 941 | CB | PRO R | 55 | | 73.751 | 6.798 | 14.112 | | | |
| | MOTA | 942 | CG | PRO R | 55 | | 72.739 | 7.924 | | 1.00 93.32 1.00 96.19 | R R | C |
| | MOTA | 943 | C | PRO R | 55 | | 73.761 | 4.774 | 15.365 | | | |
| 50 | MOTA | 944 | 0 | PRO R | 55 | | 73.823 | 5.288 | 16.474 | 1.00 96.51 | R | 0 |
| | MOTA | 945 | N | CYS R | 62 | | 71.151 | 15.108 | 19.860 | 1.00 97.98 | R | N |
| | MOTA | 946 | CA | CYS R | 62 | | 70.420 | 15.510 | 18.664 | 1.00 99.92 | R | C |
| | ATOM | 947 | С | CYS R | 62 | | 69.057 | 14.816 | 18.581 | 1.00100.12 | R | C |
| | ATOM | 948 | 0 | CYS R | 62 | | 68.951 | 13.597 | 18.581 | 1.00100.53 | R | 0 |
| 55 | ATOM | 949 | CB | CYS R | 62 | | 71.268 | 15.154 | 17.437 | 1.00100.74 | R | C |
| | ATOM | 950 | SG | CYS R | 62 | | 72.172 | 16.581 | 16.783 | 1.00104.16 | R | S |
| | ATOM | 951 | N | SER R | 63 | | 68.001 | 15.643 | 18.514 | 1.00100.26 | R | N |
| | ATOM | 952 | CA | SER R | 63 | | 66.749 | 15.214 | 17.866 | 1.00100.59 | R | C |
| | ATOM | 953 | CB | SER R | 63 | | 65.737 | 16.344 | 18.003 | 1.00100.76 | R | C |
| co | | | | | 63 | | 65.282 | 16.394 | 19.352 | 1.00100.96 | R | Ō |
| 60 | MOTA | 954 | OG C | SER R | 63 | | 66.932 | 14.883 | 16.379 | 1.00100.67 | R | č |
| | ATOM | 955 | C | SER R | | | | | 15.524 | 1.00101.08 | R | ŏ |
| | ATOM | 956 | 0 | SER R | 63 | | 67.014 | 15.751 | | | R | |
| | ATOM | 957 | N | LEU R | 64 | | 66.995 | 13.572 | 16.071 | 1.00100.07 | | И |
| | MOTA | 958 | CA | LEU R | 64 | | 67.207 | 13.155 | 14.689 | 1.00 99.22 | R | C |
| 65 | MOTA | 959 | СВ | LEU R | 64 | | 67.502 | 11.646 | 14.686 | 1.00 99.84 | R | C |
| | MOTA | 960 | CG | LEU R | 64 | | 68.992 | 11.275 | 14.695 | 1.00100.27 | R | C |
| | ATOM | 961 | CD1 | LEU R | 64 | | 69.877 | 12.258 | 13.922 | 1.00100.39 | R | C |
| | ATOM | 962 | | LEU R | 64 | | 69.562 | 11.217 | 16.105 | 1.00 99.98 | R | C |
| | MOTA | 963 | С | LEU R | 64 | | 65.974 | 13.412 | 13.822 | 1.00 98.40 | R | С |
| | | | | | | | | | | | | |

| | | | | | | | 4.4.0.40 | 1 00 00 07 | 70 | 0 |
|-----|--------------|------------------|------------------------|------------|------------------|-------------------|------------------|--------------------------|--------|--------|
| | MOTA | 964 0 | | 64 | 64.833 | 13.273 13.854 | 14.243 12.578 | 1.00 98.87 1.00 97.03 | R R | N . |
| | ATOM | 965 N | | 65 65 | 66.237 65.271 | 13.627 | 11.509 | 1.00 95.83 | R | Ĉ |
| | MOTA | 966 CF 967 CE | | 65 65 | 64.793 | 14.956 | 10.924 | 1.00 96.96 | R | С |
| 5 | ATOM ATOM | 967 CE 968 CG | | 65 | 63.709 | 15.532 | 11.742 | 1.00 97.91 | R | C |
| 5 | ATOM | | | 65 | 63.886 | 16.344 | 12.919 | 1.00 98.91 | R | C |
| | MOTA | | | 65 | 62.596 | 16.735 | 13.354 | 1.00 99.15 | R | C |
| | MOTA | | | 65 | 65.008 | 16.789 | 13.604 | 1.00 99.85 1.00 98.14 | R R | C C |
| | ATOM | | | 65 | 62.321 | 15.447 | 11.506 12.438 | 1.00 98.14 | R | N |
| 10 | MOTA | | | 65 CE | 61.599 62.463 | 16.123 17.571 | 14.454 | 1.00 99.73 | R | Ċ |
| | MOTA | | | 65 65 | 64.878 | 17.618 | 14.704 | 1.00100.22 | R | Č |
| | ATOM | | | 65 | 63.596 | 18.021 | 15.124 | 1.00100.03 | R | С |
| | ATOM ATOM | 976 CI 977 C | | 65 | 65.918 | 12.807 | 10.401 | 1.00 93.89 | R | C |
| 15 | ATOM | 978 0 | | 65 | 67.010 | 13.086 | 9.927 | 1.00 93.86 | R | 0 |
| 13 | ATOM | 979 N | | 66 | 65.219 | 11.735 | 10.013 | 1.00 91.56 | R | N |
| | ATOM | 980 C | | 66 | 65.711 | 10.896 | 8.942 | 1.00 89.74 | R R | C C |
| | MOTA | 981 C | | 66 | 65.255 | 9.461 9.052 | 9.198 10.571 | 1.00 89.58 1.00 89.53 | R | C |
| | ATOM | 982 C | | 66 | 65.678 64.721 | 8.814 | 11.553 | 1.00 89.38 | R | č |
| 20 | MOTA | | D1 TYR R E1 TYR R | 66 66 | 65.108 | 8.450 | 12.831 | 1.00 89.14 | R | C |
| | MOTA | | D2 TYR R | 66 | 67.034 | 8.931 | 10.887 | 1.00 89.34 | R | C |
| | ATOM ATOM | 200 | E2 TYR R | 66 | 67.423 | 8.576 | 12.169 | 1.00 89.67 | R | C |
| | ATOM | | Z TYR R | 66 | 66.465 | 8.343 | 13.139 | 1.00 89.51 | R | C |
| 25 | ATOM | | H TYR R | 66 | 66.843 | 8.009 | 14.424 | 1.00 88.93 | R R | 0 C |
| | MOTA | 989 C | | 66 | 65.211 | 11.378 | 7.577 7.369 | 1.00 88.13 1.00 87.44 | R | ŏ |
| | MOTA | 990 O | | 66 | 64.039 | 11.673 11.526 | 6.644 | 1.00 87.17 | R | N |
| | MOTA | 991 N | | 67 67 | 66.168 65.773 | 11.892 | 5.291 | 1.00 86.53 | R | C |
| 00 | MOTA | | A PHE R B PHE R | 67 | 66.753 | 12.949 | 4.779 | 1.00 87.70 | R | C |
| 30 | ATOM ATOM | | G PHE R | 67 | 67.092 | 13.919 | 5.872 | 1.00 89.87 | R | C |
| | ATOM | | D1 PHE R | 67 | 68.425 | 14.185 | 6.150 | 1.00 90.91 | R | C |
| | ATOM | | D2 PHE R | 67 | 66.089 | 14.643 | 6.492 | 1.00 90.84 | R | C |
| | ATOM | | CE1 PHE R | 67 | 68.756 | 15.197 | 7.037 | 1.00 90.97 1.00 91.55 | R R | C |
| 35 | MOTA | | CE2 PHE R | 67 | 66.426 | 15.660 15.945 | 7.381 7.653 | 1.00 91.55 1.00 90.84 | R | č |
| | MOTA | | ZZ PHE R | 67 67 | 67.760 65.810 | 10.660 | 4.373 | 1.00 85.67 | R | Č |
| • | MOTA | 1000 C | | 67 | 66.804 | 9.959 | 4.298 | 1.00 85.43 | R | 0 |
| | ATOM ATOM | 1001 | _ | 68 | 64.677 | 10.389 | 3.691 | 1.00 84.85 | R | N |
| 40 | ATOM | | CA SER R | 68 | 64.632 | 9.172 | 2.883 | 1.00 84.40 | R | C |
| -10 | ATOM | | CB SER R | 68 | 63.905 | 8.097 | 3.686 | 1.00 83.55 | R R | C O |
| | ATOM | 1005 | OG SER R | 68 | 62.503 | 8.380 | 3.682 | 1.00 81.92 1.00 84.96 | R R | C |
| | ATOM | | SER R | 68 | 63.983 | $9.341 \\ 10.181$ | 1.491 1.265 | 1.00 84.40 | R | ŏ |
| | ATOM | | O SER R N HIS R | 68 69 | 63.129 64.445 | 8.481 | 0.525 | 1.00 86.02 | R | N |
| 45 | MOTA | | N HIS R CA HIS R | 69 | 63.828 | 8.461 | -0.821 | 1.00 87.66 | R | С |
| | ATOM ATOM | | CB HIS R | 69 | 64.392 | 9.619 | -1.656 | 1.00 86.85 | R | C |
| | ATOM | | CG HIS R | 69 | 65.902 | 9.628 | -1.623 | 1.00 87.47 | R | C |
| | MOTA | | CD2 HIS R | 69 | 66.787 | 9.563 | -2.709 | 1.00 87.58 1.00 87.25 | R R | C N |
| 50 | MOTA | | ND1 HIS R | 69 | 66.610 | 9.974 | -0.520 -0.934 | 1.00 87.23 | R | C |
| | MOTA | | CE1 HIS R | 69 | 67.883 68.019 | 10.130 9.890 | -2.239 | 1.00 87.47 | R | N |
| | MOTA | | NE2 HIS R C HIS R | 69 69 | 64.012 | 7.121 | -1.574 | 1.00 88.70 | R | C |
| | ATOM ATOM | | O HIS R | 69 | 64.850 | | -1.242 | 1.00 88.93 | R | 0 |
| 55 | ATOM | | N PHE R | 70 | 63.154 | | -2.611 | 1.00 90.78 | R | N |
| 00 | ATOM | | CA PHE R | 70 | 63.222 | | -3.369 | 1.00 92.92 | R | C |
| | MOTA | 1020 | CB PHE R | 70 | 62.323 | | | 1.00 93.71 | R R | C |
| | MOTA | | CG PHE R | 70 | 60.965 | | -4.259 | 1.00 95.17 1.00 95.74 | R | Č |
| | MOTA | | CD1 PHE R | 70 | 60.568 | | | | R | č |
| 60 | ATOM | | CD2 PHE R CE1 PHE R | 70 70 | 60.045 59.237 | | | | R | č |
| | MOTA | | CE1 PHE R | 70 70 | 58.710 | | | | R | С |
| | ATOM | | CZ PHE R | 70 70 | 58.300 | | | 1.00 97.37 | R | C |
| | ATOM ATOM | | C PHE R | 70 | 64.654 | | -3.771 | 1.00 94.26 | R | C |
| 65 | ATOM | | O PHE R | 70 | 65.224 | | | | R | O |
| | ATOM | | N GLY R | 71 | 65.237 | | | | R R | N C |
| | ATOM | 1030 | CA GLY R | 71 | 66.672 | | | | R | C |
| | ATOM | | C GLY R | 71 71 | 67.219 68.398 | | | | R | ŏ |
| | MOTA | 1032 | O GLY R | <i>/</i> T | 102 | , ,,,,, | . 0.004 | | | |
| | | | | | 102 | | | | | |

| | | | | | | | 7 600 | 6 464 | 1 00 05 20 | TO. | λT |
|----|--------------|----------------|----------|----------------|----------|------------------|------------------|------------------|--------------------------|--------|----------|
| | ATOM | 1033 | | ASP R | 72 | 66.304 66.687 | 7.682 8.452 | -6.464 -7.620 | 1.00 95.39 1.00 94.78 | R R | С . И |
| | ATOM | 1034 | | ASP R ASP R | 72 72 | 66.031 | 7.782 | -8.819 | 1.00 95.03 | R | Ċ |
| | MOTA MOTA | 1035 1036 | | ASP R | 72 | 64.672 | 7.732 | -8.383 | 1.00 95.22 | R | č |
| 5 | ATOM | 1037 | | ASP R | 72 | 64.558 | 6.067 | -8.149 | 1.00 95.40 | R | Õ |
| J | ATOM | 1038 | | ASP R | 72 | 63.782 | 8.089 | -8.174 | 1.00 95.61 | R | 0 |
| | ATOM | 1039 | | ASP R | 72 | 66.169 | 9.821 | -7.374 | 1.00 94.54 | R | С |
| | ATOM | 1040 | | ASP R | 72 | 66.092 | 10.692 | -8.226 | 1.00 94.60 | R | 0 |
| | ATOM | 1041 | N 3 | LYS R | 73 | 65.708 | 9.868 | -6.120 | 1.00 93.66 | R | N |
| 10 | MOTA | 1042 | | LYS R | 73 | 65.465 | 11.089 | -5.397 | 1.00 92.22 | R | C |
| | MOTA | 1043 | | LYS R | 73 | 66.404 | 12.182 | -5.890 | 1.00 92.75 1.00 93.40 | R R | C |
| | MOTA | 1044 | | LYS R | 73 | 67.506 | 12.424 13.763 | -4.860 -4.135 | 1.00 93.40 | R | G |
| | ATOM | 1045 | | LYS R LYS R | 73 73 | 67.357 68.037 | 13.777 | -2.762 | 1.00 93.89 | R | Č |
| 15 | ATOM ATOM | $1046 \\ 1047$ | | LYS R | 73 73 | 69.488 | 13.668 | -2.911 | 1.00 92.82 | R | N |
| 15 | ATOM | 1048 | | LYS R | 73 | 64.001 | 11.473 | -5.442 | 1.00 90.85 | R | С |
| | ATOM | 1049 | | LYS R | 73 | 63.600 | 12.621 | -5.317 | 1.00 90.69 | R | 0 |
| | MOTA | 1050 | | GLN R | 74 | 63.228 | 10.393 | -5.600 | 1.00 89.30 | R | N |
| | ATOM | 1051 | | GLN R | 74 | 61.805 | 10.441 | -5.868 | 1.00 87.34 | R | C |
| 20 | ATOM | 1052 | | GLN R | 74 | 61.606 | 9.323 | -6.899 -7.787 | 1.00 88.25 1.00 89.67 | R R | C |
| | MOTA | 1053 | | GLN R | 74 74 | 60.377 60.643 | 9.479 8.798 | -7.787 -9.116 | 1.00 89.67 | R | Č |
| | MOTA MOTA | 1054 1055 | _ | GLN R GLN R | 74 74 | 61.026 | | -10.103 | 1.00 92.95 | R | ŏ |
| | ATOM | 1056 | | GLN R | 74 | 60.357 | 7.480 | -9.127 | 1.00 91.90 | R | N |
| 25 | ATOM | 1057 | | GLN R | 74 | 61.033 | 10.092 | -4.588 | 1.00 85.48 | R | C |
| | ATOM | 1058 | 0 | GLN R | 74 | 61.214 | 9.035 | -4.000 | 1.00 85.72 | R | 0 |
| | ATOM | 1059 | | ASP R | 75 | 60.185 | 11.039 | -4.128 | 1.00 83.23 | R | N |
| | ATOM | 1060 | | ASP R | 75 | 59.332 | 10.746 | -2.983 | 1.00 80.16 1.00 82.21 | R R | C |
| 00 | ATOM | 1061 | | ASP R | 75 75 | 58.981 57.502 | 9.261 9.096 | -3.011 -3.338 | 1.00 82.21 | R | Ċ |
| 30 | ATOM ATOM | 1062 1063 | | ASP R ASP R | 75 75 | 57.164 | 9.141 | -4.521 | 1.00 85.14 | R | Ö |
| | ATOM | 1063 | | ASP R | 75 75 | 56.720 | 8.862 | -2.420 | 1.00 84.69 | R | 0 |
| | ATOM | 1065 | | ASP R | 75 | 60.041 | 11.078 | -1.661 | 1.00 77.76 | R | C |
| | ATOM | 1066 | 0 | ASP R | 75 | 60.008 | 10.338 | -0.685 | 1.00 76.11 | R | 0 |
| 35 | MOTA | 1067 | | LYS R | 76 | 60.715 | 12.247 | -1.666 | 1.00 75.72 | R | N |
| | ATOM | 1068 | | LYS R | 76 | 61.444 | 12.689 | -0.481 | 1.00 73.28 1.00 73.94 | R R | C |
| | MOTA | 1069 | | LYS R | 76 76 | 62.046 63.136 | 14.065 14.004 | -0.791 -1.863 | 1.00 73.94 | R | C |
| | ATOM ATOM | 1070 1071 | | LYS R | 76 76 | 63.136 | 15.285 | -1.911 | 1.00 73.77 | R | č |
| 40 | ATOM | 1071 | | LYS R | 76 76 | 63.143 | 16.510 | -2.309 | 1.00 74.55 | R | C |
| 40 | ATOM | 1073 | - | LYS R | 76 | 62.828 | 16.449 | -3.735 | 1.00 75.61 | R | N |
| | ATOM | 1074 | | LYS R | 76 | 60.526 | 12.788 | 0.730 | 1.00 72.29 | R | C |
| | MOTA | 1075 | - | LYS R | 76 | 59.350 | 13.111 | 0.637 | 1.00 71.88 | R | 0 |
| | ATOM | 1076 | | LYS R | 77 | 61.096 | 12.452 12.588 | 1.902 | 1.00 70.63 1.00 69.48 | R R | N C |
| 45 | ATOM | 1077 1078 | | LYS R | 77 77 | 60.330 59.496 | 11.319 | 3.133 3.333 | 1.00 67.92 | R | č |
| | ATOM ATOM | 1078 | | LYS R | 77 | 58.863 | 11.259 | 4.727 | 1.00 67.24 | R | č |
| | ATOM | 1080 | | LYS R | 77 | 57.814 | 10.153 | 4.846 | 1.00 66.40 | R | С |
| | ATOM | 1081 | | LYS R | 77 | 56.879 | 10.358 | 6.044 | 1.00 66.77 | R | C |
| 50 | MOTA | 1082 | NZ | LYS R | 77 | 55.637 | 9.616 | 5.830 | 1.00 67.40 | R | Ŋ |
| | MOTA | 1083 | C | LYS R | 77 | 61.247 | 12.796 | 4.340 | 1.00 69.93 | R | C |
| | MOTA | 1084 | 0 | LYS R | 77 | 62.297 | 12.187 13.727 | $4.479 \\ 5.215$ | 1.00 70.78 1.00 69.90 | R R | N O |
| | MOTA | 1085 | N CA | ILE R | 78 78 | 60.836 61.586 | 13.727 | 6.450 | 1.00 69.33 | R | Ĉ |
| 55 | ATOM ATOM | 1086 1087 | CB | ILE R | 78 | 62.195 | 15.319 | 6.435 | 1.00 70.19 | R | č |
| 33 | MOTA | 1088 | | ILE R | 78 | 63.156 | 15.475 | 7.627 | 1.00 70.90 | R | C |
| | ATOM | 1089 | | ILE R | 78 | 63.001 | 15.527 | 5.152 | 1.00 70.70 | R | С |
| | ATOM | 1090 | | ILE R | 78 | 63.489 | 16.969 | 5.006 | 1.00 68.74 | R | C |
| | MOTA | 1091 | C | ILE R | 78 | 60.694 | 13.746 | 7.680 | 1.00 68.68 | R | C |
| 60 | ATOM | 1092 | 0 | ILE R | 78 70 | 59.701 | 14.435 | 7.869 | 1.00 67.88 1.00 68.91 | R R | N O |
| | MOTA | 1093 | N | ALA R | 79 79 | 61.060 60.281 | 12.756 12.512 | 8.517 9.724 | 1.00 68.91 | R R | C |
| | MOTA | 1094 1095 | CA CB | ALA R ALA R | 79 79 | 59.107 | 11.601 | 9.724 | 1.00 68.88 | R | Č |
| • | MOTA MOTA | 1095 | CP | ALA R | 79 79 | 61.129 | 11.860 | 10.819 | 1.00 70.08 | R | č |
| 65 | ATOM | 1097 | Ö | ALA R | 79 | 62.184 | 11.289 | 10.576 | 1.00 69.58 | R | 0 |
| | MOTA | 1098 | N | PRO R | 80 | 60.650 | 11.997 | 12.070 | 1.00 70.73 | R | N |
| | ATOM | 1099 | CD | PRO R | 80 | 59.418 | 12.638 | 12.493 | 1.00 70.72 | R | C |
| | MOTA | 1100 | CA | PRO R | | 61.365 | 11.478 | 13.228 | 1.00 71.37 1.00 71.34 | R R | C |
| | MOTA | 1101 | CB | PRO R | 80 | 60.674 | 12.013 | 14.482 | T.00 /T.34 | Х | C |
| | | | | | | 104 | | | | | |

| | ATOM ATOM | 1102 1103 | CG C | PRO R PRO R | 80 80 | 59.556 61.366 | 12.963 9.949 | 14.052 13.255 | 1.00 71.52 1.00 71.72 | | R R | C |
|------|--------------|---------------------|------------|------------------|----------|------------------|-----------------------|------------------|--------------------------|---|--------|--------|
| | ATOM | 1104 | 0 | PRO R | 80 | 62.344 | 9.298 9.377 | 13.601 12.912 | 1.00 71.37 1.00 71.96 | | R R | N O |
| 5 | ATOM ATOM | 1105 1106 | N CA | GLU R GLU R | 81 81 | 60.199 60.060 | 7.929 | 12.912 | 1.00 71.90 | | R | C |
| 5 | ATOM | 1107 | CB | GLU R | 81 | 58.701 | 7.554 | 12.380 | 1.00 71.77 | | R | C |
| | ATOM | 1108 | C | GLU R | 81 | 61.171 | 7.213 | 12.203 | 1.00 72.33 | | R | C |
| | MOTA | 1109 | 0 | GLU R | 81 | 61.605 61.668 | 7.627 6.121 | 11.135 12.812 | 1.00 72.11 1.00 73.39 | | R R | O N |
| 10 | ATOM ATOM | $1110 \\ 1111$ | N CA | THR R THR R | 82 82 | 62.630 | 5.283 | 12.109 | 1.00 74.33 | | R | C |
| 10 | ATOM | 1112 | CB | THR R | 82 | 63.531 | 4.607 | 13.136 | 1.00 75.38 | | R | C |
| | ATOM | 1113 | OG1 | THR R | 82 | 62.729 | 3.844 | 14.038 | 1.00 76.17 | | R | 0 |
| | MOTA | 1114 | CG2 | THR R | 82 | 64.298 | 5.669 4.218 | 13.929 11.297 | 1.00 75.33 1.00 73.70 | | R R | C |
| 45 | MOTA MOTA | 1115 1116 | С О | THR R | 82 82 | 61.892 62.164 | 3.028 | 11.357 | 1.00 73.70 | | R | ŏ |
| 15 | ATOM | 1117 | N | ARG R | 83 | 60.895 | 4.714 | 10.537 | 1.00 73.78 | | R | N |
| | ATOM | 1118 | CA | ARG R | 83 | 59.978 | 3.835 | 9.819 | 1.00 73.66 | | R | C |
| | MOTA | 1119 | CB | ARG R | 83 | 58.786 58.272 | $3.593 \\ 2.154$ | 10.749 10.702 | 1.00 74.64 1.00 76.22 | | R R | C |
| 20 | MOTA MOTA | 1120 1121 | CG CD | ARG R ARG R | 83 83 | 57.196 | 1.978 | 9.629 | 1.00 78.40 | | R | č |
| 20 | ATOM | 1122 | NE | ARG R | 83 | 55.847 | 1.899 | 10.201 | 1.00 79.66 | | R | N |
| | MOTA | 1123 | CZ | ARG R | 83 | 54.934 | 2.805 | 9.789 | 1.00 80.93 | | R | C |
| | ATOM | 1124 | NH1 | | 83 | 55.312 53.636 | $3.854 \\ 2.491$ | 9.074 9.860 | 1.00 80.54 1.00 80.52 | | R R | N |
| O.F. | ATOM ATOM | 1125 1126 | NH2 C | ARG R ARG R | 83 83 | 59.488 | 4.525 | 8.542 | 1.00 30.32 | | R | Č |
| 25 | ATOM | 1127 | ŏ | ARG R | 83 | 59.068 | 5.673 | 8.542 | 1.00 72.88 | | R | 0 |
| | MOTA | 1128 | N | ARG R | 84 | 59.598 | 3.805 | 7.411 | 1.00 70.90 | | R | N |
| | MOTA | 1129 | CA | ARG R | 84 | 59.031 60.154 | 4.353 4.823 | 6.185 5.262 | 1.00 69.83 1.00 69.23 | | R R | C |
| 30 | ATOM ATOM | 1130 1131 | CB CG | ARG R ARG R | 84 84 | 59.604 | 5.431 | 3.202 | 1.00 68.67 | | R | Č |
| 30 | ATOM | 1132 | CD | ARG R | 84 | 59.507 | 6.960 | 4.043 | 1.00 69.89 | | R | C |
| | MOTA | 1133 | NE | ARG R | 84 | 58.601 | 7.472 | 3.010 | 1.00 67.69 | | R | N |
| | MOTA | 1134 | CZ | ARG R | 84 | 59.154 | 8.160 8.357 | 1.996 1.963 | 1.00 66.16 1.00 63.97 | | R R | C N |
| 35 | ATOM ATOM | 1135 1136 | | ARG R | 84 84 | 60.460 58.380 | 8.621 | 1.008 | 1.00 66.32 | | R | N |
| 33 | ATOM | 1137 | C | ARG R | 84 | 58.157 | 3.337 | 5.458 | 1.00 69.55 | | R | C |
| | ATOM | 1138 | 0 | ARG R | 84 | 58.625 | 2.376 | 4.863 | 1.00 68.26 | | R | 0 |
| | MOTA | 1139 | N | SER R | 85 | 56.836 55.906 | 3.565 2.676 | 5.554 4.881 | 1.00 69.16 1.00 69.24 | | R R | N C |
| 40 | ATOM ATOM | $1140 \\ 1141$ | CA CB | SER R SER R | 85 85 | 54.733 | 2.413 | 5.824 | 1.00 68.28 | | R | Č |
| 40 | ATOM | 1142 | OG | SER R | 85 | 53.828 | 1.499 | 5.204 | 1.00 66.67 | | R | 0 |
| | MOTA | 1143 | С | SER R | 85 | 55.396 | 3.283 | 3.574 | 1.00 69.39 1.00 69.33 | | R R | C |
| | MOTA | 1144 | O | SER R ILE R | 85 86 | 55.016 55.437 | $\frac{4.444}{2.458}$ | 3.493 2.511 | 1.00 69.33 | | R | N |
| 45 | ATOM ATOM | $\frac{1145}{1146}$ | N CA | ILE R | 86 | 54.972 | 2.933 | 1.215 | 1.00 71.79 | | R | С |
| 40 | ATOM | 1147 | CB | ILE R | 86 | 56.195 | 3.312 | 0.379 | 1.00 71.58 | • | Ř | C |
| | MOTA | 1148 | CG2 | | 86 | 55.744 | 3.879 | -0.979 1.094 | 1.00 72.31 | | R R | C |
| | MOTA | 1149 1150 | CG1 CD1 | | 86 86 | 57.003 58.384 | 4.399 4.603 | 0.470 | 1.00 71.33 1.00 72.37 | | R | Č |
| 50 | MOTA MOTA | 1151 | C CD3 | ILE R | 86 | 54.144 | 1.872 | 0.488 | 1.00 72.39 | | R | С |
| | MOTA | 1152 | 0 | ILE R | 86 | 54.496 | 0.701 | 0.413 | 1.00 73.22 | | R | O |
| | MOTA | 1153 | N | GLU R | 87 | 52.979 | 2.317 | -0.019 -0.758 | 1.00 73.42 1.00 74.10 | | R R | С И |
| | ATOM ATOM | 1154 1155 | CA CB | GLU R GLU R | 87 87 | 52.108 50.672 | $\frac{1.411}{1.900}$ | -0.736 | 1.00 73.40 | | R | Č |
| 55 | ATOM | 1156 | CG | GLU R | | 49.632 | 0.876 | -1.028 | 1.00 75.07 | | R | C |
| - | ATOM | 1157 | CD | GLU R | | 48.275 | 1.302 | -0.517 | 1.00 75.32 | | R | C |
| | ATOM | 1158 | | L GLU R | | 47.877 | 0.841 2.136 | 0.543 -1.165 | 1.00 76.51 1.00 74.90 | | R R | 0 |
| | MOTA MOTA | 1159 1160 | OE2 C | 2 GLU R GLU R | | 47.644 52.467 | 1.398 | -2.246 | 1.00 75.06 | | R | č |
| 60 | ATOM | 1161 | Ö | GLU R | | 51.997 | 2.201 | -3.041 | 1.00 75.38 | | R | 0 |
| | ATOM | 1162 | N | VAL R | . 88 | 53.367 | 0.464 | -2.601 | 1.00 76.09 | | R | N |
| | MOTA | 1163 | CA | VAL R | | 53.874 | $0.431 \\ 0.746$ | -3.967 -3.908 | 1.00 77.64 1.00 77.48 | | R R | C |
| | ATOM ATOM | 1164 1165 | CB CB | VAL R 1 VAL R | | 55.369 56.029 | 0.746 | -5.245 | 1.00 77.35 | | R | C |
| 65 | ATOM | 1166 | | 2 VAL R | | 55.580 | 2.216 | -3.591 | 1.00 78.41 | | R | С |
| = = | MOTA | 1167 | С | VAL R | . 88 | 53.667 | -0.949 | -4.611 | 1.00 78.83 | | R | C |
| | MOTA | 1168 | O | VAL R | | 53.779 53.310 | -1.982 -0.918 | -3.975 -5.909 | 1.00 79.09 1.00 79.58 | | R R | O N |
| | ATOM ATOM | 1169 1170 | N CD | PRO R PRO R | | 53.310 | 0.231 | | 1.00 79.45 | | R | Ĉ |
| | Y TOM | ,0 | ر. ت | _ 1.0 1 | | | | | | | | |

| | ATOM ATOM | 1171 1172 | CA CB | PRO R PRO R | 89 89 | 53.177 52.607 | -2.154 -1.797 | -6.677 -8.049 | 1.00 80.36 1.00 79.98 | R R | C |
|-----|---------------|---------------------|------------|------------------|----------|------------------|-------------------|--------------------|--------------------------|--------|--------|
| | MOTA | 1173 | CG | PRO R | 89 | 52.642 | -0.279 | -8.214 -6.830 | 1.00 80.10 1.00 80.61 | R R | C |
| _ | ATOM ATOM | 1174 1175 | C O | PRO R PRO R | 89 89 | 54.529 55.539 | -2.853 -2.256 | -7.177 | 1.00 80.05 | R | Ö |
| 5 | ATOM | 1176 | N | LEU R | 90 | 54.535 | -4.163 | -6.517 | 1.00 82.18 | R | N |
| | ATOM | 1177 | CA | LEU R | 90 | 55.798 | -4.893 | -6.473 | 1.00 83.61 | R R | C |
| | ATOM | 1178 | CB | LEU R | 90 | 55.669 56.915 | -5.986 -6.102 | -5.411 -4.531 | 1.00 83.45 1.00 83.26 | R | C |
| 10 | ATOM ATOM | 1179 1180 | CG CD1 | LEU R LEU R | 90 90 | 58.057 | -5.205 | -5.012 | 1.00 82.85 | R | C |
| 10 | ATOM | 1181 | CD2 | LEU R | 90 | 56.649 | -5.716 | -3.077 | 1.00 83.25 | R | C |
| | MOTA | 1182 | C | LEU R | 90 | 56.149 | -5.531 | -7.818 | 1.00 84.45 | R | C |
| | MOTA | 1183 | 0 | LEU R | 90 | 56.305 | -6.740 -4.678 | -7.946 -8.851 | 1.00 84.45 1.00 85.73 | R R | N O |
| 45 | ATOM ATOM | $\frac{1184}{1185}$ | N CA | ASN R ASN R | 91 91 | 56.249 56.525 | | -10.180 | 1.00 86.79 | R | C |
| 15 | ATOM | 1186 | CB | ASN R | 91 | 55.775 | -4.350 | -11.198 | 1.00 87.26 | R | C |
| | ATOM | 1187 | CG | ASN R | 91 | 54.294 | | -11.082 | 1.00 87.64 | R R | C |
| | ATOM | 1188 | | ASN R | 91 | 53.855 53.504 | -5.727 -3.552 | -10.799 -11.309 | 1.00 88.26 1.00 88.14 | R | N |
| 20 | MOTA MOTA | 1189 1190 | ND2 C | ASN R ASN R | 91 91 | 58.026 | -5.224 | -10.486 | 1.00 87.60 | R | C |
| 20 | ATOM | 1191 | Ö | ASN R | 91 | 58.464 | -5.525 | -11.588 | 1.00 87.91 | R | 0 |
| | MOTA | 1192 | N | GLU R | 92 | 58.824 | -4.841 | -9.468 | 1.00 88.44 | R R | N C |
| | MOTA | 1193 | CA | GLU R | 92 | 60.272 60.628 | -4.903 -4.319 | -9.638 -11.005 | 1.00 89.44 1.00 91.03 | R | C |
| OF. | MOTA MOTA | 1194 1195 | CB CG | GLU R GLU R | 92 92 | 60.945 | -2.825 | -10.947 | 1.00 92.82 | R | C |
| 25 | ATOM | 1196 | CD | GLU R | 92 | 60.923 | -2.262 | -12.349 | 1.00 94.79 | R | C |
| | MOTA | 1197 | OE1 | | 92 | 61.180 | -1.078 | -12.510 | 1.00 95.91 | R R | 0 |
| | MOTA | 1198 | OE2 | | 92 | 60.644 61.038 | -3.020 -4.180 | -13.277 -8.523 | 1.00 95.77 1.00 89.16 | R | č |
| 30 | ATOM ATOM | 1199 1200 | C O | GLU R GLU R | 92 92 | 60.486 | -3.467 | -7.695 | 1.00 89.19 | R | 0 |
| 30 | ATOM | 1201 | N | ARG R | 93 | 62.364 | -4.423 | -8.510 | 1.00 88.70 | R | N |
| | MOTA | 1202 | CA | ARG R | 93 | 63.203 | -3.932 | -7.420 | 1.00 88.39 | R R | C |
| | ATOM | 1203 | CB | ARG R | 93 | 64.665 62.939 | -4.113 -2.465 | -7.829 -7.066 | 1.00 87.82 1.00 87.79 | R | C |
| 05 | ATOM ATOM | $\frac{1204}{1205}$ | C | ARG R ARG R | 93 93 | 62.856 | -1.587 | -7.915 | 1.00 87.40 | R | ō |
| 35 | ATOM | 1205 | N | ILE R | 94 | 62.769 | -2.230 | -5.749 | 1.00 87.29 | R | N |
| | ATOM | 1207 | CA | ILE R | 94 | 62.664 | -0.862 | -5.252 | 1.00 86.37 | R R | C |
| | MOTA | 1208 | CB | ILE R | 94 | 61.253 61.094 | -0.652 0.802 | -4.696 -4.220 | 1.00 86.45 1.00 86.59 | R | Č |
| 40 | MOTA MOTA | $\frac{1209}{1210}$ | CG2 CG1 | | 94 94 | 60.207 | -0.907 | -5.784 | 1.00 86.32 | R | С |
| 40 | ATOM | 1211 | CD1 | | 94 | 58.881 | -1.413 | -5.208 | 1.00 86.05 | R | C |
| | ATOM | 1212 | C | ILE R | 94 | 63.695 | -0.604 | -4.147 | 1.00 85.38 1.00 84.68 | R R | C |
| | MOTA | 1213 | 0 | ILE R | 94 95 | 63.836 64.457 | $-1.364 \\ 0.492$ | -3.198 -4.319 | 1.00 85.21 | R | N |
| 45 | ATOM ATOM | $1214 \\ 1215$ | N CA | CYS R CYS R | 95 95 | 65.507 | 0.790 | -3.358 | 1.00 85.65 | R | C |
| 45 | ATOM | 1216 | C | CYS R | | 65.252 | 2.112 | -2.629 | 1.00 85.09 | R | C |
| | MOTA | 1217 | 0 | CYS R | 95 | 64.956 | 3.144 | -3.216 | 1.00 86.18 | R R | C |
| | MOTA | 1218 | CB SG | CYS R CYS R | | 66.840 67.232 | 0.862 -0.692 | -4.097 -4.935 | 1.00 85.94 1.00 87.89 | R | s |
| 50 | $oxdot{MOTA}$ | 1219 1220 | N | LEU R | | 65.336 | 2.029 | -1.288 | 1.00 83.68 | R | N |
| 00 | MOTA | 1221 | CA | LEU R | 96 | 65.177 | 3.219 | | 1.00 82.89 | R | C |
| | MOTA | 1222 | CB | LEU R | | 64.174 | 2.881 4.096 | | 1.00 83.32 1.00 84.29 | R R | C |
| | MOTA | $\frac{1223}{1224}$ | CG CD1 | LEU R L LEU R | | 63.814 62.885 | 3.732 | | 1.00 84.58 | R | С |
| 55 | ATOM ATOM | 1225 | | LEU R | | 65.036 | 4.766 | 2.130 | 1.00 84.50 | R | C |
| - | ATOM | 1226 | C | LEU R | 96 | 66.513 | 3.625 | | 1.00 82.63 | R | C |
| | ATOM | 1227 | 0 | LEU R | | 67.326 | 2.802 | | 1.00 82.88 1.00 81.96 | R R | N |
| | MOTA | 1228 | N CA | GLN R GLN R | | 66.746 67.965 | 4.949 5.448 | | 1.00 81.67 | R | Ĉ |
| 60 | ATOM ATOM | 1229 1230 | CB | GLN R | | 68.768 | 6.217 | | 1.00 82.00 | R | С |
| | ATOM | 1231 | CG | GLN R | . 97 | 68.849 | 5.471 | _1.553 | 1.00 83.05 | R | C |
| | MOTA | 1232 | CD | GLN R | | 69.895 | 6.119 7.298 | | 1.00 84.66 1.00 85.58 | R R | C |
| | MOTA | 1233 1234 | OE: | | | 70.197 70.450 | 5.278 | | 1.00 85.66 | R | N |
| 65 | MOTA MOTA | 1234 | | GLN R | | 67.641 | 6.363 | 2.015 | 1.00 81.37 | R | С |
| 00 | ATOM | 1236 | 0 | GLN R | 97 | 66.796 | 7.246 | 1.945 | 1.00 81.46 | R | O |
| | ATOM | 1237 | N | VAL F | | 68.323 | 6.104 6.848 | | 1.00 80.64 1.00 80.06 | R R | N C |
| | MOTA | 1238 1239 | | VAL F VAL F | | 67.991 67.544 | 5.854 | | 1.00 79.37 | R | č |
| | ATOM | 1433 | دري | A 7-7-1 | .) | | | _ | | | |

| | ATOM | 1240 | CG1 | VAL R | 98 | 67.098 | 6.608 | 6.681 | 1.00 79.32 | R | С |
|----|--------------|---------------------|----------|----------------|-------------|------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM | 1241 | | VAL R | 98 | 66.385 | 5.026 | 4.909 | 1.00 78.50 | R | C |
| | ATOM | 1242 | C | VAL R | 98 | 69.157 70.318 | 7.690 7.298 | 4.880 4.862 | 1.00 81.16 1.00 81.24 | R R | C O |
| 5 | ATOM ATOM | $\frac{1243}{1244}$ | N O | VAL R GLY R | 98 99 | 68.812 | 8.909 | 5.331 | 1.00 81.88 | R | И |
| 5 | ATOM | 1245 | CA | GLY R | 99 | 69.837 | 9.776 | 5.891 | 1.00 82.68 | R | С |
| | ATOM | 1246 | С | GLY R | 99 | 69.464 | 10.232 | 7.305 | 1.00 84.10 | R | C |
| | ATOM | 1247 | 0 | GLY R | 99 | 68.411 | 9.924 | 7.841 | 1.00 83.64 | R | 0 |
| | ATOM | 1248 | N | SER R | | 70.396 | 10.959 11.415 | 7.931 9.284 | 1.00 85.90 1.00 87.83 | R R | N C |
| 10 | ATOM ATOM | 1249 1250 | CA CB | SER R SER R | | 70.121 70.710 | 10.397 | 10.265 | 1.00 87.83 | R | Č |
| | ATOM | 1251 | OG | SER R | | 71.800 | 9.715 | 9.644 | 1.00 88.31 | R | ŏ |
| | ATOM | 1252 | C | SER R | 100 | 70.709 | 12.796 | 9.550 | 1.00 89.25 | R | C |
| | ATOM | 1253 | 0 | SER R | 100 | 71.786 | 13.162 | 9.082 | 1.00 89.46 | R | 0 |
| 15 | MOTA | 1254 | N | GLN R | | 69.936 | 13.598 | 10.288 | 1.00 91.48 | R | N |
| | ATOM | 1255 | CA | GLN R GLN R | | 70.425 70.213 | 14.879 15.904 | 10.717 9.576 | 1.00 93.60 1.00 94.44 | R R | C |
| | ATOM ATOM | 1256 1257 | CB CG | GLN R | | 71.127 | 17.132 | 9.692 | 1.00 96.46 | R | Č |
| | ATOM | 1258 | CD | GLN R | | 71.264 | 17.819 | 8.347 | 1.00 98.38 | R | Ċ |
| 20 | MOTA | 1259 | OE1 | _ | | 72.104 | 18.676 | 8.125 | 1.00 98.68 | R | 0 |
| | MOTA | 1260 | NE2 | | | 70.364 | 17.416 | 7.428 | 1.00 99.02 | R | N |
| | ATOM | 1261 | C | GLN R | | 69.730 | 15.338 | 11.984 12.548 | 1.00 94.64 1.00 94.60 | R R | C |
| | ATOM | 1262 1263 | N O | GLN R CYS R | | 68.847 70.231 | 14.680 16.468 | 12.548 | 1.00 94.00 | R | N |
| 25 | MOTA MOTA | 1264 | CA | CYS R | | 69.461 | 17.283 | 13.413 | 1.00 98.14 | R | Ĉ |
| 20 | ATOM | 1265 | C | CYS R | | 68.847 | 18.509 | 12.703 | 1.00 98.53 | R | C |
| | MOTA | 1266 | 0 | CYS R | | 69.462 | 19.202 | 11.916 | 1.00 98.75 | R | 0 |
| | ATOM | 1267 | CB | CYS R | | 70.380 | 17.718 | 14.572 | 1.00100.07 | R R | C S |
| 00 | MOTA | 1268 | SG | CYS R SER R | | 71.772 67.548 | 16.589 18.696 | 14.795 12.995 | 1.00103.24 1.00 98.95 | R R | N |
| 30 | MOTA MOTA | 1269 1270 | N CA | SER R | | 66.595 | 19.624 | 12.355 | 1.00 99.38 | R | Ĉ |
| | ATOM | 1271 | CB | SER R | | 66.606 | 20.940 | 13.115 | 1.00 98.08 | R | C |
| | ATOM | 1272 | OG | SER R | | 65.536 | 20.923 | 14.065 | 1.00 96.68 | R | 0 |
| | MOTA | 1273 | C | SER R | | 66.688 | 19.831 | 10.821 | 1.00 99.93 | R | C |
| 35 | MOTA | 1274 | 0 | SER R | | 67.649 | 20.353 19.195 | 10.244 10.439 | 1.00 99.98 1.00 99.96 | R R | N O |
| | MOTA MOTA | 1275 1276 | CA N | THR R | | 65.642 65.032 | 19.704 | 9.178 | 1.00 99.76 | R | C |
| | ATOM | 1277 | CB | THR R | | 64.043 | 20.795 | 9.529 | 1.00100.10 | R | Č |
| | ATOM | 1278 | č | THR R | | 66.026 | 20.149 | 8.072 | 1.00100.47 | R | C |
| 40 | MOTA | 1279 | 0 | THR R | | 65.699 | 20.769 | 7.076 | 1.00100.37 | R | 0 |
| | MOTA | 1280 | ·N | ASN R | | 67.276 | 19.782 | 7.996 | 1.00100.21 | Ŕ | N |
| | MOTA | 1281 | CA | ASN R | | 68.419 69.653 | 20.151 19.323 | 7.115 7.589 | 1.00 99.27 1.00 97.89 | R R | C |
| | MOTA MOTA | 1282 1283 | CB | ASN R ASN R | | 68.288 | 19.916 | 5.567 | 1.00 99.40 | R | č |
| 45 | MOTA | 1284 | ŏ | ASN R | | 67.455 | 19.207 | 5.023 | 1.00100.19 | R | 0 |
| | MOTA | 1285 | N | PRO R | | 72.314 | 16.855 | 4.636 | 1.00100.55 | R | N |
| | MOTA | 1286 | CA | PRO R | | 72.840 | 15.913 | 5.617 | 1.00100.45 | R | C |
| | MOTA | 1287 | CB | PRO R | | 71.986 | 14.672 15.072 | 5.770 5.036 | 1.00101.19 1.00101.27 | R R | C |
| 50 | MOTA MOTA | 1288 1289 | C C | PRO R PRO R | | 73.978 74.344 | 15.403 | 3.916 | 1.00101.62 | R | ŏ |
| 50 | ATOM | 1290 | И | SER R | | 74.750 | 14.116 | 5.919 | 1.00100.19 | R | N |
| | MOTA | 1291 | CA | SER R | 111 | 75.399 | 13.143 | 5.074 | 1.00 99.29 | R | C |
| | MOTA | 1292 | CB | SER R | | 76.872 | 13.512 | 4.960 | 1.00 97.71 | R | C |
| | MOTA | 1293 | C | SER R | | 75.341 | 11.764 11.461 | 5.668 6.807 | 1.00 98.69 1.00 98.52 | R R | C |
| 55 | MOTA MOTA | 1294 1295 | N O | SER R ILE R | | 75.754 74.746 | 10.922 | 4.840 | 1.00 99.04 | R | N |
| | MOTA | 1296 | CA | ILE R | | 75.165 | 9.539 | 4.751 | 1.00 99.58 | R | C |
| | MOTA | 1297 | CB | ILE R | | 76.692 | 9.451 | 4.699 | 1.00 99.70 | R | С |
| | MOTA | 1298 | C | ILE R | | 74.419 | 8.805 | 3.609 | 1.00 99.23 | R | C |
| 60 | MOTA | 1299 | 0 | ILE R | | 74.281 | 9.299 | 2.486 | 1.00100.32 1.00 97.67 | R | O M |
| | MOTA | 1300 | N | LEU R | | 73.927 72.906 | 7.616 7.051 | 3.933 3.045 | 1.00 97.67 | R R | N C |
| | MOTA MOTA | 1301 1302 | CA CB | LEU R LEU R | 113 | 72.900 | 7.791 | 1.691 | 1.00 93.23 | R | Č |
| | ATOM | 1302 | CG | LEU R | 113 | 72.331 | 9.214 | 1.777 | 1.00 92.82 | R | С |
| 65 | ATOM | 1304 | CD1 | L LEU R | 113 | 71.476 | 9.616 | 0.561 | 1.00 91.70 | R | C |
| | MOTA | 1305 | | LEU R | | 71.410 | 9.399 | 3.013 | 1.00 91.48 | R | C |
| | ATOM | 1306 | C | LEU R | | 73.160 | 5.560 | 2.873 2.154 | 1.00 93.45 1.00 93.20 | R R | C |
| | ATOM | 1307 1308 | N O | LEU R VAL R | 11 <i>/</i> | 74.056 72.380 | 5.139 4.736 | 3.637 | 1.00 93.20 | R | И |
| | ATOM | 7200 | TA | A 5277 7/ | | , 2.500 | 2.750 | 2.337 | | | |

| | | | | | | | | | | _ | |
|----|--------------|--------------|----------|------------------------|------------------|--------------------|-------------------|--------------------------|------------|--------|--------|
| | ATOM | 1309 | CA V | VAL R 114 | 72.514 | 3.279 | 3.525 | 1.00 90.61 | | R R | C C |
| | MOTA | | | VAL R 114 | 72.534 | 2.706 | 4.935 | 1.00 89.74 1.00 89.47 | E 7 | R | C |
| | MOTA | | | VAL R 114 | 72.373 | 3.859 1.750 | 5.915 5.134 | 1.00 88.54 | | R | Č |
| | MOTA | | | VAL R 114 | 71.374 71.342 | 2.683 | 2.746 | 1.00 90.72 | | R | Ċ |
| 5 | MOTA | | | VAL R 114 | 70.199 | 2.822 | 3.164 | 1.00 91.38 | | R | 0 |
| | ATOM | | O] | VAL R 114 GLU R 115 | 71.712 | 2.188 | 1.554 | 1.00 90.13 | 3 | R | N |
| | ATOM | | N | GLU R 115 | 70.695 | 1.671 | 0.650 | 1.00 89.00 | | R | C |
| | ATOM | | CA CB | GLU R 115 | 71.318 | | -0.742 | 1.00 89.83 | | R | C |
| 10 | ATOM ATOM | | | GLU R 115 | 70.350 | | -1.858 | 1.00 92.8 | | R | C |
| 10 | ATOM | | | GLU R 115 | 71.063 | | -3.189 | 1.00 94.83 | | R | C |
| | ATOM | | OE1 | GLU R 115 | 72.217 | | -3.213 | 1.00 95.98 | | R R | 0 |
| | ATOM | | | GLU R 115 | 70.456 | 2.217 | -4.199 | 1.00 96.13 1.00 87.3 | | R R | C |
| | MOTA | | | GLU R 115 | 70.185 | 0.306 | 1.110 1.660 | 1.00 87.3 | | R | ŏ |
| 15 | ATOM | 1323 | | GLU R 115 | 70.909 | -0.514 0.096 | 0.916 | 1.00 85.6 | | R | Ň |
| | MOTA | | | LYS R 116 | 68.874 68.332 | -1.235 | 1.126 | 1.00 84.1 | 7 | R | С |
| | ATOM | 1325 | | LYS R 116 LYS R 116 | 67.757 | -1.337 | 2.534 | 1.00 83.5 | | R | С |
| | MOTA | 1326 | | LYS R 116 | 67.431 | -2.785 | 2.904 | 1.00 83.4 | 4 | R | С |
| 00 | MOTA | 1327 1328 | CD | LYS R 116 | 67.624 | -3.735 | 1.718 | 1.00 84.4 | | R | C |
| 20 | ATOM ATOM | 1329 | CE | LYS R 116 | 68.553 | -4.910 | 2.046 | 1.00 85.5 | | R | C |
| | ATOM | 1330 | NZ | LYS R 116 | 69.779 | -4.808 | 1.255 | 1.00 85.5 | | R | C N |
| | MOTA | 1331 | С | LYS R 116 | 67.248 | -1.545 | 0.097 | 1.00 83.7 | 3 7 · | R R | Ö |
| | MOTA | 1332 | 0 | LYS R 116 | 66.214 | -0.904 | $0.017 \\ -0.747$ | 1.00 83.6 1.00 83.5 | 2 | R | N |
| 25 | ATOM | 1333 | N | CYS R 117 | 67.530 | -2.544 -2.801 | -1.795 | 1.00 83.4 | | R | C |
| | MOTA | 1334 | CA | CYS R 117 | 66.550 65.652 | -3.988 | -1.441 | 1.00 82.8 | | R | С |
| | MOTA | 1335 | C | CYS R 117 CYS R 117 | 65.897 | -4.726 | -0.495 | 1.00 82.3 | | R | 0 |
| | MOTA | 1336 1337 | O CB | CYS R 117 | 67.306 | -3.088 | -3.094 | 1.00 84.0 | 2 | R | C |
| 20 | ATOM ATOM | 1338 | SG | CYS R 117 | 68.355 | -1.705 | -3.595 | 1.00 86.0 | | R | s |
| 30 | ATOM | 1339 | N | ILE R 118 | 64.545 | -4.039 | -2.208 | 1.00 82.7 | | R | N |
| | MOTA | 1340 | CA | ILE R 118 | 63.714 | -5.216 | -2.171 | 1.00 82.4 | | R | C C |
| | ATOM | 1341 | СВ | ILE R 118 | 62.480 | -5.009 | -1.286 | 1.00 81.3 1.00 80.8 | | R R | C |
| | MOTA | 1342 | CG2 | | 61.646 | -3.807 | -1.763 -1.436 | 1.00 80.7 | | R | Č |
| 35 | MOTA | 1343 | CG1 | | 61.620 | -6.260 -6.308 | -0.523 | 1.00 80.7 | | R | Č |
| | MOTA | 1344 | CD1 | | 60.414 63.304 | -5.663 | -3.565 | 1.00 83.5 | | R | C |
| | MOTA | 1345 | C | ILE R 118 ILE R 118 | 62.966 | -4.886 | -4.439 | 1.00 82.6 | 58 | R | 0 |
| | MOTA | 1346 1347 | N O | SER R 119 | 63.361 | -6.981 | -3.749 | 1.00 85.3 | 39 | R | N |
| 40 | MOTA MOTA | 1348 | CA | SER R 119 | 63.152 | -7.476 | -5.110 | 1.00 87.6 | | R | C |
| 40 | MOTA | 1349 | CB | SER R 119 | 64.288 | -8.446 | -5.451 | 1.00 87.4 | | R | C |
| | MOTA | 1350 | OG | SER R 119 | 65.357 | -7.750 | -6.088 | 1.00 88.6 | 04 11 | R R | O C |
| | MOTA | 1351 | С | SER R 119 | 61.834 | -8.220 | -5.234 | 1.00 89.3 1.00 89.3 | 1.1 2.7 | R | Ö |
| | MOTA | 1352 | 0 | SER R 119 | 61.298 | -8.757 -8.233 | -4.272 -6.467 | 1.00 90. | 5.5 | R | Ň |
| 45 | MOTA | 1353 | N | PRO R 120 | 61.292 61.793 | -7.579 | -7.673 | 1.00 90. | | R | C |
| | MOTA | 1354 | CD | PRO R 120 PRO R 120 | 60.061 | -8.965 | -6.760 | 1.00 91. | | R | С |
| | MOTA | 1355 1356 | CA CB | PRO R 120 | 59.837 | -8.901 | -8.271 | 1.00 91. | 34 | R | С |
| | MOTA ATOM | 1357 | CG | PRO R 120 | 61.078 | -8.283 | -8.926 | 1.00 90. | 81 | R | C |
| 50 | ATOM | 1358 | C | PRO R 120 | 60.195 | -10.427 | -6.337 | 1.00 93. | 40 | R | C |
| 00 | ATOM | 1359 | Õ | PRO R 120 | 61.246 | -10.897 | -5.963 | 1.00 93. | ον 2Τ | R R | O N |
| | ATOM | 1360 | N | PRO R 121 | 59.052 | -11.126 | -6.319 | 1.00 94. 1.00 95. | | R | C |
| | ATOM | 1361 | CD | PRO R 121 | 57.679 | -10.642 | -6.320 -6.186 | | | R | Č |
| | ATOM | 1362 | CA | PRO R 121 | 59.U3I | -12.588 -13.050 | -6.133 | | | R | C |
| 55 | ATOM | 1363 | CB | PRO R 121 | 57.363 | -11.825 | -5.792 | | | R | С |
| | MOTA | 1364 | CG | PRO R 121 PRO R 121 | 59 710 | -13.314 | -7.354 | 1.00 96. | 27 | R | C |
| | MOTA | 1365 1366 | C | PRO R 121 | 60.232 | -12.728 | -8.290 | 1.00 96. | 65 | R | 0 |
| | MOTA MOTA | 1367 | N | GLU R 122 | 59.712 | -14.654 | -7.263 | 1.00 96. | | R | N |
| 60 | MOTA | 1368 | CA | GLU R 122 | 60.466 | -15.436 | -8.239 | | 64 | R | C |
| 00 | MOTA | 1369 | CB | GLU R 122 | 60.754 | -16.811 | -7.647 | 1.00 98. | TΩ | R | C |
| | MOTA | 1370 | C | GLU R 122 | 59.750 | -15.566 | -9.580 | | 0.3 1.6 | R R | 0 |
| | ATOM | 1371 | 0 | GLU R 122 | 58.765 | -14.900 | -9.861 | 1.00 98. 1.00 98. | 3.3 T.0 | R | N |
| | MOTA | 1372 | N | GLY R 123 | 60.290 | -16.456 -16.367 | -11 Q/A | | 34 | R | Ĉ |
| 65 | MOTA | 1373 | CA | | 59.903 | -16.367 -14.924 | -12 276 | | 41 | R | Č |
| | ATOM | 1374 | | GLY R 123 GLY R 123 | 60.036 | -14.096 | -11.527 | 1.00 97. | 99 | R | 0 |
| | ATOM | 1375 1376 | | ASP R 124 | 59.740 | -14.604 | -13.517 | 1.00 98. | 66 | R | N |
| | ATOM ATOM | 1377 | | 401 | 59.442 | -15.503 | -14.620 | 1.00 98. | .83 | R | С |
| | A 1 OM | ±317 | O£1 | | 108 | | | | | | |

| | | | | | _ | - |
|-----|--------------|------------------|--------------------------------|--|--------|--------|
| | ATOM | 1378 C | B ASP K 124 | 59.960 -16.929 -14.423 1.00 98.61 59.663 -14.888 -15.999 1.00 98.97 | R R | C C |
| | ATOM | 1379 C | 404 | 59 298 -15.411 -17.040 1.00 98.84 | R | 0 |
| | ATOM ATOM | 1380 O 1381 N | PRO R 125 | 60.276 - 13.683 - 15.943 1.00 99.06 | R R | N C |
| 5 | ATOM | 1382 C | D PRO R 125 | 60.842 -13.053 -14.762 1.00 99.07 60.488 -12.806 -17.076 1.00 99.15 | R | C |
| | MOTA | | A PRO R 125 B PRO R 125 | 61.557 -11.780 -16.757 1.00 98.98 | R | C |
| | MOTA MOTA | | G PRO R 125 | 61.684 -11.758 -15.228 1.00 99.03 | R R | C |
| | MOTA | 1386 C | PRO R 125 | 59.183 -12.245 -17.658 1.00 98.89 58.874 -11.068 -17.541 1.00 98.69 | R | ŏ |
| 10 | MOTA | 1387 C | | 58.446 -13.145 -18.351 1.00 98.52 | R | N |
| | ATOM ATOM | | CA GLUR 126 | 57.012 -12.938 -18.505 1.00 98.29 | R R | C C |
| | ATOM | 1390 C | CB GLU R 126 | 56.502 -13.566 -19.812 1.00 99.27 56.541 -12.662 -21.043 1.00102.26 | R | C |
| | MOTA | | CG GLU R 126 CD GLU R 126 | 55.852 -11.335 -20.795 1.00105.09 | R | C |
| 15 | ATOM ATOM | | DE1 GLU R 126 | 54.628 -11.301 -20.704 1.00106.59 | R R | 0 |
| | ATOM | 1394 (| DE2 GLU R 126 | 56.540 -10.316 -20.869 1.00105.98 56.272 -13.649 -17.392 1.00 97.16 | R | Č |
| | MOTA | | C GLU R 126 C GLU R 126 | 56.659 -13.635 -16.227 1.00 97.88 | R | 0 |
| 20 | ATOM ATOM | | N SER R 127 | 55.187 -14.322 -17.835 1.00 95.40 | R R | N C |
| 20 | MOTA | | CA SER R 127 | 54.401 -15.089 -16.897 1.00 93.82 55.389 -15.802 -15.987 1.00 93.96 | R | č |
| | MOTA | | CB SER R 127 OG SER R 127 | 56.514 -14.940 -15.779 1.00 94.37 | R | 0 |
| | ATOM ATOM | | C SER R 127 | 53.518 -14.151 -16.082 1.00 92.55 52.410 -14.462 -15.681 1.00 92.49 | R R | C |
| 25 | MOTA | | O SER R 127 | 52.410 -14.462 -15.681 1.00 92.49 54.072 -12.966 -15.792 1.00 91.22 | R | N |
| | MOTA MOTA | | N ALA R 128 CA ALA R 128 | 53.280 -11.874 -15.294 1.00 89.83 | R | C |
| | ATOM | | CB ALA R 128 | 54.233 -10.749 -14.877 1.00 90.27 52.291 -11.385 -16.357 1.00 89.00 | R R | C |
| | MOTA | | C ALA R 128 O ALA R 128 | 52.291 -11.385 -16.357 1.00 89.00 52.593 -11.270 -17.547 1.00 89.71 | R | 0 |
| 30 | MOTA MOTA | | O ALA R 128 N VAL R 129 | 51.043 -11.174 -15.890 1.00 87.77 | R R | N C |
| | MOTA | | CA VAL R 129 | 50.001 -10.665 -16.765 1.00 86.32 48.672 -10.733 -16.005 1.00 86.35 | R | C |
| | MOTA | | CB VAL R 129 CG1 VAL R 129 | 48 937 -11.160 -14.558 1.00 86.60 | R | C |
| 35 | MOTA MOTA | | CG2 VAL R 129 | 48.001 -9.372 -16.008 1.00 87.18 | R R | C C |
| 33 | ATOM | | C VAL R 129 | 50.293 -9.209 -17.159 1.00 84.92 51.181 -8.563 -16.623 1.00 84.48 | R | Ö |
| | ATOM | 1414 | O VAL R 129 N THR R 130 | 49 543 -8.723 -18.164 1.00 83.78 | R | N |
| | ATOM ATOM | 1415 1416 | CA THR R 130 | 49.720 -7.344 -18.604 1.00 83.06 | R R | C |
| 40 | MOTA | 1417 | CB THR R 130 | 50.487 -7.341 -19.933 1.00 83.42 49.697 -7.975 -20.935 1.00 85.56 | R | ŏ |
| | MOTA | 1418 1419 | OG1 THR R 130 CG2 THR R 130 | 51.791 -8.120 -19.765 1.00 84.04 | R | C |
| | MOTA MOTA | 1420 | C THR R 130 | 48.388 -6.605 -18.755 1.00 82.58 47.346 -7 176 -19.059 1.00 81.67 | R R | C |
| | ATOM | 1421 | O THR R 130 | 47.346 -7.176 -19.059 1.00 81.67 48.453 -5.287 -18.472 1.00 82.27 | R | N |
| 45 | MOTA MOTA | 1422 1423 | N GLU R 131 CA GLU R 131 | 47.280 -4.438 -18.639 1.00 81.66 | R | C |
| | ATOM | 1424 | CB GLU R 131 | 46.754 -4.623 -20.063 1.00 84.16 47.786 -4.215 -21.115 1.00 87.93 | R R | C |
| | ATOM | 1425 | CG GLU R 131 CD GLU R 131 | 47.786 -4.215 -21.115 1.00 87.93 47.177 -4.323 -22.494 1.00 89.79 | R | С |
| 50 | MOTA MOTA | 1426 1427 | OE1 GLU R 131 | 46.187 -5.025 -22.643 1.00 91.97 | R R | 0 |
| 50 | ATOM | 1428 | OE2 GLU R 131 | 47.707 -3.706 -23.417 1.00 90.84 46.192 -4.785 -17.621 1.00 79.25 | R | č |
| | MOTA | 1429 | C GLU R 131 O GLU R 131 | 45.052 -5.087 -17.952 1.00 78.94 | R | 0 |
| | ATOM ATOM | 1430 1431 | N LEU R 132 | 46.601 - 4.772 - 16.340 1.00 76.59 | R R | N C |
| 55 | MOTA | 1432 | CA LEU R 132 | 45.667 -5.109 -15.275 1.00 74.32 46.444 -5.852 -14.186 1.00 72.56 | R | С |
| | MOTA | 1433 1434 | CB LEU R 132 CG LEU R 132 | 45.695 -5.895 -12.852 1.00 72.22 | R | C |
| | MOTA MOTA | 1435 | CD1 LEU R 132 | 44.557 -6.918 -12.857 1.00 70.16 | R R | C C |
| | MOTA | 1436 | CD2 LEU R 132 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | R | Č |
| 60 | MOTA | 1437 1438 | C LEU R 132 O LEU R 132 | 45.555 -3.191 -13.812 1.00 73.40 | R | 0 |
| | MOTA MOTA | 1439 | N GLN R 133 | 43.829 -3.521 -15.225 1.00 74.00 | R R | N C |
| | MOTA | 1440 | CA GLN R 133 | 42 967 -1.312 -15.759 1.00 76.12 | R | С |
| e E | MOTA | | CB GLN R 133 CG GLN R 133 | 42.873 -1.889 -17.172 1.00 79.10 | R | C |
| 65 | ATOM ATOM | | CD GLN R 133 | 43.181 -0.798 -18.172 1.00 81.25 | R R | C |
| | ATOM | 1444 | OE1 GLN R 133 | 44 499 -0.562 -18.329 1.00 81.66 | R | N |
| | ATOM ATOM | | NE2 GLN R 133 C GLN R 133 | 41.702 -2.801 -14.184 1.00 71.52 | R | С |
| | AIOM | . 1770 | <u> </u> | 100 | | |

| ATOM ATOM ATOM | 1447 1448 1449 | N CYS R 134 CA CYS R 134 | 41.232 39.920 | -3.744 -14.665 -2.078 -13.152 -2.382 -12.597 | 1.00 72.04 1.00 68.85 1.00 66.75 | R R R | С И О |
|------------------------------|--|---|--|---|--|------------------------|---|
| ATOM ATOM ATOM ATOM | 1451 1452 1453 | O CYS R 134 CB CYS R 134 SG CYS R 134 | 39.351 40.101 41.160 | -0.096 -13.109 -2.704 -11.113 -4.144 -10.850 | 1.00 63.78 1.00 68.38 1.00 70.34 | R R R | 0 C S |
| ATOM ATOM ATOM ATOM | 1454 1455 1456 1457 | CA ILE R 135 CB ILE R 135 | 36.651 35.924 34.513 | -0.466 -12.585 -0.554 -13.929 0.051 -13.804 | 1.00 58.36 1.00 57.94 1.00 54.74 | R R R | N C |
| ATOM ATOM ATOM | 1458 1459 1460 | CD1 ILE R 135 C ILE R 135 | 36.044 35.652 | 0.094 -16.383 -0.668 -11.443 | 1.00 58.96 1.00 57.95 | R R R R | 0000 |
| ATOM ATOM ATOM | 1462 1463 1464 | N TRP R 136 CA TRP R 136 CB TRP R 136 | 35.325 34.426 34.890 | 0.439 -10.754 0.325 -9.612 1.306 -8.532 | 1.00 56.24 1.00 56.61 1.00 55.50 | R R R | и С С |
| ATOM ATOM ATOM ATOM | 1465 1466 1467 1468 | CD2 TRP R 136 CE2 TRP R 136 | 34.362 33.698 | 1.749 -6.011 1.024 -4.991 3.007 -5.728 | 1.00 54.02 1.00 54.07 1.00 55.35 | R R R | CC |
| ATOM ATOM ATOM | 1469 1470 1471 | NE1 TRP R 130 CZ2 TRP R 130 | 33.229 33.579 | -0.260 -5.572 1.569 -3.722 | 1.00 54.86 1.00 54.29 | R R | C N C |
| ATOM ATOM ATOM | 1473 1474 1475 | CH2 TRP R 130 C TRP R 130 O TRP R 130 | 34.101 32.972 32.566 | 2.830 -3.454 0.614 -10.000 1.751 -10.199 | 1.00 54.57 1.00 56.90 1.00 58.05 | R R R | C C |
| ATOM ATOM ATOM | 1477 1478 | CA HIS R 13' CB HIS R 13' | 30.800 30.303 | -0.466 -10.142 -0.300 -10.621 -1.640 -11.161 -1.874 -12.533 | 1.00 56.91 1.00 56.03 1.00 55.23 1.00 54.71 | R R R | N C C |
| MOTA MOTA MOTA | 1480 1481 1482 | CD2 HIS R 13' ND1 HIS R 13' CE1 HIS R 13' | 7 30.191 7 32.201 7 32.312 | -2.030 -13.744 -2.030 -12.764 -2.281 -14.080 | 1.00 55.22 1.00 55.84 1.00 55.03 | R R R | C N C N |
| MOTA MOTA | 1484 1485 1486 | C HIS R 13 | 7 29.840 7 29.586 | $ \begin{array}{rrr} 0.183 & -9.529 \\ -0.487 & -8.535 \\ 1.415 & -9.739 \end{array} $ | 1.00 56.49 1.00 58.18 1.00 56.21 | R R R | 0 C |
| MOTA ATOM MOTA | 1487 1488 1489 | CB ASN R 13 CG ASN R 13 | 26.999 25.749 | $ \begin{array}{rrr} 1.050 & -9.197 \\ 1.805 & -8.827 \end{array} $ | 1.00 57.44 1.00 58.23 1.00 60.13 | R R | 0 0 0 0 |
| ATOM ATOM ATOM ATOM | 1491 1492 1493 | ND2 ASN R 13 C ASN R 13 O ASN R 13 | 8 25.729 8 28.559 8 27.689 | 3.095 -9.205 1.952 -7.426 1.976 -6.563 | 1.00 59.12 1.00 58.33 1.00 57.09 | R R R | И С О |
| ATOM ATOM ATOM | 1494 1495 1496 | CA LEU R 13 CB LEU R 13 | 9 30.374 9 29.862 | 1.919 -5.763 3.163 -5.020 | 1.00 60.87 1.00 59.70 | R R | И С С |
| MOTA MOTA | 1498 1499 1500 | CD1 LEU R 13 CD2 LEU R 13 C LEU R 13 | 9 29.998 9 31.841 9 29.939 | 5.673 -4.669 4.582 -5.839 0.651 -5.005 | 1.00 57.96 1.00 58.45 1.00 62.49 | R R R | C C C |
| MOTA MOTA | 1502 1503 | N SER R 14 CA SER R 14 | 0 29.775 0 29.161 | -0.460 -5.765 -1.676 -5.226 | 1.00 63.81 1.00 65.20 | R R R | О И С С |
| ATOM ATOM ATOM | 1505 1506 1507 | OG SER R 14 C SER R 14 O SER R 14 | 0 26.752 0 30.048 0 30.173 | -1.372 -5.276 -2.920 -5.404 -3.762 -4.521 | 1.00 68.36 1.00 65.22 1.00 66.71 | R R R | 0 C 0 |
| MOTA MOTA MOTA | 1509 1510 | CA TYR R 14 CB TYR R 14 | 1 31.504 1 30.764 | -4.140 -6.975 $-5.360 -7.555$ | 1.00 64.42 1.00 65.04 | R R R R | N C D |
| ATOM ATOM ATOM | 1512 1513 1514 | CD1 TYR R 14 CE1 TYR R 14 CD2 TYR R 14 | 1 31.014 1 30.470 1 28.984 | -5.507 -10.064 -5.399 -11.345 -4.600 -9.136 | 1.00 66.95 1.00 67.61 1.00 67.12 | R R R R | 0000 |
| | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | ATOM 1448 ATOM 1449 ATOM 1450 ATOM 1451 ATOM 1453 ATOM 1453 ATOM 1455 ATOM 1455 ATOM 1455 ATOM 1455 ATOM 1456 ATOM 1457 ATOM 1458 ATOM 1460 ATOM 1461 ATOM 1462 ATOM 1463 ATOM 1463 ATOM 1466 ATOM 1466 ATOM 1466 ATOM 1467 ATOM 1468 ATOM 1469 ATOM 1470 ATOM 1471 ATOM 1472 ATOM 1473 ATOM 1474 ATOM 1475 ATOM 1478 ATOM 1478 ATOM 1480 ATOM 1481 ATOM 1482 ATOM 1483 ATOM 1484 ATOM 1488 ATOM 1488 ATOM 1488 ATOM 1488 ATOM 1488 ATOM 1489 ATOM 1490 ATOM 1491 ATOM 1491 ATOM 1492 ATOM 1493 ATOM 1496 ATOM 1497 ATOM 1497 ATOM 1497 ATOM 1498 ATOM 1498 ATOM 1499 ATOM 1491 ATOM 1491 ATOM 1491 ATOM 1492 ATOM 1493 ATOM 1496 ATOM 1497 ATOM 1497 ATOM 1497 ATOM 1498 ATOM 1499 ATOM 1500 ATOM 1501 ATOM 1501 ATOM 1508 ATOM 1508 ATOM 1509 ATOM 1509 ATOM 1501 | ATOM 1448 N CYS R 134 ATOM 1449 CA CYS R 134 ATOM 1450 C CYS R 134 ATOM 1451 O CYS R 134 ATOM 1451 O CYS R 134 ATOM 1452 CB CYS R 134 ATOM 1453 SG CYS R 134 ATOM 1455 CA LLE R 135 ATOM 1455 CA LLE R 135 ATOM 1456 CB ILE R 135 ATOM 1457 CG2 ILE R 135 ATOM 1457 CG2 ILE R 135 ATOM 1459 CD1 ILE R 135 ATOM 1450 C ILE R 135 ATOM 1461 O ILE R 135 ATOM 1461 O ILE R 135 ATOM 1462 CB TRP R 136 ATOM 1463 CA TRP R 136 ATOM 1464 CB TRP R 136 ATOM 1465 CG TRP R 136 ATOM 1466 CD2 TRP R 136 ATOM 1466 CD2 TRP R 136 ATOM 1467 CE2 TRP R 136 ATOM 1469 CD1 TRP R 136 ATOM 1470 NE1 TRP R 136 ATOM 1470 NE1 TRP R 136 ATOM 1471 CZZ TRP R 136 ATOM 1472 CZZ TRP R 136 ATOM 1474 C TRP R 136 ATOM 1476 N HIS R 137 ATOM 1478 CB HIS R 137 ATOM 1481 ND1 HIS R 137 ATOM 1482 CE1 HIS R 137 ATOM 1484 C HIS R 137 ATOM 1485 O HIS R 137 ATOM 1486 CB ASN R 138 ATOM 1487 CA ASN R 138 ATOM 1488 CB ASN R 138 ATOM 1489 CG ASN R 138 ATOM 1490 OD1 ASN R 138 ATOM 1491 ND2 ASN R 138 ATOM 1492 C ASN R 138 ATOM 1493 O ASN R 138 ATOM 1494 N LEU R 13 ATOM 1496 CB LEU R 13 ATOM 1497 CG LEU R 13 ATOM 1498 CD1 LEU R 13 ATOM 1499 CD2 LEU R 13 ATOM 1499 CD2 LEU R 13 ATOM 1499 CD2 LEU R 13 ATOM 1490 CD3 ASN R 138 ATOM 1496 CB SER R 14 ATOM 1500 C LEU R 13 ATOM 1497 CG LEU R 13 ATOM 1498 CD1 LEU R 13 ATOM 1498 CD1 LEU R 13 ATOM 1498 CD1 LEU R 13 ATOM 1496 CB SER R 14 ATOM 1500 C SER R 14 ATOM 1500 | ATOM 1448 N CYS R 134 41.232 ATOM 1449 CA CYS R 134 39.920 ATOM 1451 O CYS R 134 39.351 ATOM 1451 O CYS R 134 40.101 ATOM 1453 SG CYS R 134 41.160 ATOM 1454 N LLE R 135 37.670 ATOM 1455 CA LLE R 135 37.670 ATOM 1455 CA LLE R 135 36.651 ATOM 1455 CA LLE R 135 36.651 ATOM 1455 CB LLE R 135 36.651 ATOM 1455 CB LLE R 135 36.661 ATOM 1455 CB LLE R 135 36.661 ATOM 1455 CB LLE R 135 36.6684 ATOM 1459 CD1 LLE R 135 36.6684 ATOM 1459 CD1 LLE R 135 36.6684 ATOM 1465 CB LLE R 135 35.221 ATOM 1461 O LLE R 135 35.221 ATOM 1462 N TRP R 136 35.325 ATOM 1465 CG TRP R 136 34.890 ATOM 1465 CG TRP R 136 34.890 ATOM 1466 CD2 TRP R 136 34.890 ATOM 1466 CD2 TRP R 136 34.890 ATOM 1467 CE2 TRP R 136 33.698 ATOM 1469 CD1 TRP R 136 33.698 ATOM 1469 CD1 TRP R 136 33.698 ATOM 1470 NE1 TRP R 136 33.229 ATOM 1471 CZ2 TRP R 136 33.693 ATOM 1470 NE1 TRP R 136 33.229 ATOM 1471 CZ2 TRP R 136 33.229 ATOM 1474 C TRP R 136 32.972 ATOM 1475 O TRP R 136 32.972 ATOM 1476 N HIS R 137 30.800 ATOM 1477 CA HIS R 137 30.800 ATOM 1478 CB HIS R 137 30.801 ATOM 1488 CB LEU R 139 ATOM 1488 CB ATOM 1489 CD HIS R 137 30.8975 ATOM 1488 CB ASN R 138 26.999 ATOM 1488 CB ASN R 138 26.999 ATOM 1489 CD ASN R 138 26.999 ATOM 1489 CD ASN R 138 26.999 ATOM 1499 CD ASN R 138 26.999 ATOM 1499 CD ASN R 138 26.999 ATOM 1499 CD ASN R 138 27.689 ATOM 1499 CD LEU R 139 30.344 ATOM 1495 CA EEU R 139 30.374 ATOM 1496 CB LEU R 139 30.374 ATOM 1497 CG SER R 140 29.775 ATOM 1490 CD ASN R 138 26.999 ATOM 1491 CO ASN R 138 27.989 ATOM 1491 CG SER R 140 29.775 ATOM 1492 CD ASN R 138 26.999 ATOM 1493 C ASN R 138 26.999 ATOM 1496 CB LEU R 139 30.374 ATOM 1497 CG SER R 140 29.775 ATOM 1498 CD LEU R 139 30.374 ATOM 1496 CB LEU R 139 30.374 ATOM 1496 CB LEU R 139 30.374 ATOM 1496 CB LEU R 139 29.998 ATOM 1496 CB EEU R 139 30.374 ATOM 1504 CB SER R | ATOM | AROM 1449 CA CYS R 134 | AROM 1448 N CYS R 134 41.232 -2.078 -13.152 1.00 68.85 R AROM 1459 CA CYS R 134 38.950 -1.204 -12.765 1.00 64.75 R AROM 1451 O CYS R 134 38.950 -1.204 -12.765 1.00 64.75 R AROM 1451 O CYS R 134 39.951 -0.996 -13.109 1.00 63.78 R AROM 1452 CB CYS R 134 40.101 -2.704 -11.113 1.00 68.38 R AROM 1453 SG CYS R 134 40.101 -2.704 -11.113 1.00 68.38 R AROM 1454 N ILLE R 135 34.101 -4.144 -1.01 1.00 68.38 R AROM 1455 CB CYS R 134 40.101 -2.704 -11.113 1.00 68.38 R AROM 1456 N ILLE R 135 36.661 -1.046 -1.2551 1.00 58.36 R AROM 1456 CB ILLE R 135 35.96 -0.554 -1.3929 1.00 57.94 R AROM 1457 CG2 ILE R 135 34.513 0.051 -13.804 1.00 57.95 R AROM 1458 CG1 ILE R 135 36.664 0.235 -15.002 1.00 57.95 R AROM 1459 CD1 ILE R 135 36.044 0.235 -15.002 1.00 57.95 R AROM 1461 O ILE R 135 35.562 -0.668 1.1443 1.00 57.95 R AROM 1462 N TRR R 136 35.214 -1.773 -11.154 1.00 57.95 R AROM 1463 CR TRR R 136 34.406 0.335 -10.61 1.00 57.95 R AROM 1463 CR TRR R 136 34.406 0.335 -10.61 1.00 57.95 R AROM 1466 CD TRR R 136 34.406 0.335 -0.632 1.00 57.95 R AROM 1467 CC2 TRR R 136 34.408 0.335 -0.632 1.00 55.50 R AROM 1468 CG3 TRR R 136 34.436 0.335 -0.632 1.00 55.50 R AROM 1466 CD TRR R 136 34.436 0.335 -0.632 1.00 55.50 R AROM 1467 CC2 TRR R 136 34.436 0.335 -0.632 1.00 55.50 R AROM 1468 CG3 TRR R 136 34.436 1.00 5.96 -8.532 1.00 56.24 R AROM 1467 CC2 TRR R 136 34.362 1.749 -6.011 1.00 54.02 R AROM 1469 CD1 TRR R 136 33.638 1.004 -4.991 1.00 54.02 R AROM 1469 CD1 TRR R 136 33.638 1.004 0.00 57.57 R AROM 1469 CD1 TRR R 136 33.532 0.00 0.949 -6.010 1.00 54.02 R AROM 1470 CR3 TRR R 136 33.509 0.00 0.99 -1.00 54.02 R AROM 1470 CR3 TRR R 136 33.509 0.00 0.99 -1.00 57.00 57.50 R AROM 1470 CR3 TRR R 136 33.656 I.00 0.00 57.57 R AROM 1470 CR3 TRR R 136 33.500 0.00 0.00 0.00 0.00 57.50 5.00 R AROM 1470 CR3 TRR R 136 33.500 0.00 0.00 0.00 0.00 57.50 5.00 R AROM 1470 CR3 TRR R 136 33.500 0.00 0.00 0.00 0.00 55.00 58.05 R AROM 1470 CR3 TRR R 136 33.500 0.00 0.00 0.00 0.00 55.00 58.05 R AROM 1470 CR3 TRR R 136 33.500 0.00 0.00 0.00 0.00 55.00 58.05 R AROM 1470 CR3 |

| | ATOM ATOM ATOM | 1516 CZ 1517 OH 1518 C | | 29.187 -4.867 -11.512 1.00 69.06 R 28.686 -4.663 -12.784 1.00 70.63 R 32.562 -3.673 -7.969 1.00 64.10 R | 0 C |
|----|--------------------------------------|--|--|---|--------------------------|
| 5 | ATOM ATOM ATOM ATOM | 1519 O 1520 N 1521 CA 1522 CB | TYR R 141 MET R 142 MET R 142 | 32.363 -2.768 -8.768 1.00 62.44 R 33.729 -4.322 -7.860 1.00 63.99 R 34.866 -3.989 -8.702 1.00 65.48 R 36.087 -3.829 -7.792 1.00 67.21 R | . N . C . C |
| 10 | ATOM ATOM ATOM ATOM ATOM | 1522 CG 1524 SE 1525 CE 1526 C | MET R 142 MET R 142 MET R 142 MET R 142 | 37.378 -3.604 -8.578 1.00 70.81 R 38.408 -2.330 -7.838 1.00 77.72 R 37.167 -1.030 -7.767 1.00 73.36 R 35.114 -5.094 -9.727 1.00 66.17 R 35.148 -6.274 -9.414 1.00 66.91 | . s . c |
| | ATOM ATOM ATOM | 1527 O 1528 N 1529 CF | | 35.148 -6.274 -9.414 1.00 66.91 35.228 -4.675 -10.996 1.00 66.36 35.483 -5.639 -12.054 1.00 67.05 34.401 -5.434 -13.123 1.00 67.92 | R N R C |
| 15 | ATOM ATOM ATOM ATOM | 1530 CF 1531 CC 1532 CF 1533 CF | G LYS R 143 D LYS R 143 | 34.352 -6.571 -14.136 1.00 69.19 34.202 -6.060 -15.569 1.00 71.27 33.224 -6.905 -16.390 1.00 71.16 | 2 C |
| 20 | MOTA ATOM ATOM ATOM ATOM | 1534 NZ 1535 C 1536 O 1537 N | LYS R 143 LYS R 143 LYS R 143 | 36.885 -5.425 -12.641 1.00 66.66 37.241 -4.354 -13.113 1.00 65.97 37.717 -6.477 -12.519 1.00 67.07 | R C R O R N |
| 25 | MOTA MOTA MOTA | 1538 C 1539 C 1540 O | A CYS R 144 CYS R 144 CYS R 144 | 39.334 -7.295 -14.192 1.00 68.24 38.754 -8.366 -14.315 1.00 68.16 40.022 -6.762 -11.845 1.00 68.98 | R C R C R C |
| | ATOM ATOM ATOM ATOM | 1541 C 1542 S 1543 N 1544 C | G CYS R 144 SER R 145 A SER R 145 | 39.869 -5.642 -10.436 1.00 71.30 40.189 -6.811 -15.106 1.00 69.43 40.555 -7.578 -16.284 1.00 71.06 | R S R N R C R C |
| 30 | ATOM ATOM ATOM ATOM | | 1 1 5 | 38.849 -6.438 -17.578 1.00 70.80 42.055 -7.818 -16.286 1.00 73.04 42.769 -7.484 -15.352 1.00 74.36 | R O R C R O |
| 35 | MOTA MOTA MOTA | 1549 N 1550 C 1551 C | TRP R 146 CA TRP R 146 CB TRP R 146 | 43.959 -8.386 -17.558 1.00 76.46 44.624 -8.758 -16.236 1.00 74.01 | R Ñ R C R C R C |
| 40 | ATOM ATOM ATOM ATOM | 1553 C 1554 C 1555 C | CD2 TRP R 146 CE2 TRP R 146 CE3 TRP R 146 | 43.481 -10.743 -14.999 1.00 70.76 43.658 -12.150 -14.994 1.00 69.26 42.532 -10.170 -14.162 1.00 69.78 | R C R C R C R C |
| | MOTA MOTA MOTA | 1557 N 1558 C | CD1 TRP R 146 NE1 TRP R 146 CZ2 TRP R 146 CZ3 TRP R 146 | 44.718 -12.484 -15.980 1.00 69.89 42.907 -12.940 -14.138 1.00 69.54 41.777 -10.959 -13.310 1.00 70.52 | R N R C R C |
| 45 | MOTA MOTA MOTA MOTA | 1560 C 1561 C | CH2 TRP R 146 C TRP R 146 O TRP R 146 | 41.967 -12.353 -13.296 1.00 70.22 44.364 -9.384 -18.607 1.00 78.90 43.596 -10.217 -19.071 1.00 78.80 | R C R C R O R N |
| 50 | ATOM ATOM ATOM | 1563 I 1564 0 1565 0 | N LEU R 147 CA LEU R 147 CB LEU R 147 CG LEU R 147 | 46.095 -10.155 -20.040 1.00 84.15 46.536 -9.336 -21.253 1.00 84.22 45.336 -8.822 -22.059 1.00 84.97 | R C R C R C |
| | MOTA MOTA MOTA | 1567 1568 | CD1 LEU R 147 CD2 LEU R 147 C LEU R 147 | 45.717 -7.748 -23.080 1.00 84.53 44.630 -9.929 -22.834 1.00 84.27 47.217 -11.057 -19.564 1.00 85.74 | R C R C R C R O |
| 55 | MOTA MOTA MOTA | 1571 1572 | O LEU R 147 N PRO R 148 CD PRO R 148 CA PRO R 148 | 47.344 -12.163 -20.303 1.00 87.39 46.558 -12.564 -21.455 1.00 87.86 48 403 -13.171 -20.129 1.00 88.19 | R N R C R C |
| 60 | MOTA MOTA MOTA MOTA | 1574 1575 | CB PRO R 148 CG PRO R 148 C PRO R 148 | 47.965 -14.454 -20.828 1.00 88.40 46.691 -14.155 -21.610 1.00 88.42 49.756 -12.659 -20.686 1.00 89.62 | R C R C R C R O |
| | MOTA MOTA MOTA | 1577 1578 1579 | O PRO R 148 N GLY R 149 CA GLY R 149 | 49.806 -11.662 -21.387 | R N R C R C |
| 65 | MOTA MOTA MOTA MOTA | 1581 1582 1583 | O GLY R 149 N ARG R 150 CA ARG R 150 | 54.234 -12.169 -21.354 1.00 94.74 53.062 -13.955 -22.026 1.00 93.01 54.181 -14.608 -22.661 1.00 92.26 | R O R N R C R C |
| | MOTA | | CB ARG R 150 | 54.955 -13.873 -23.754 1.00 91.41 | - |

| | ATOM ATOM | 1585 1586 | C ARG R 15 O ARG R 15 | | -16.106 -16.717 | | 1.00 91.84 1.00 92.36 | R R | C 0 |
|----|--------------|--------------|------------------------------|-----------|--------------------|--------------------|--------------------------|--------|--------|
| | ATOM | 1587 | N THR R 15 | | | -21.738 -21.146 | 1.00 90.45 1.00 89.19 | R R | N C |
| 5 | ATOM ATOM | 1588 1589 | CA THR R 15 | | -18.215 | -19.955 | 1.00 88.80 | R | G |
| Ū | ATOM | 1590 | C THR R 15 | 1 53.030 | -17.751 | | 1.00 87.94 | R | C |
| | MOTA | 1591 1592 | O THR R 15 N ASN R 15 | 1 52.703 | -17.915 -21.051 | -19.507 | 1.00 88.05 1.00 85.88 | R R | NO |
| | ATOM ATOM | 1592 | N ASN R 15 CA ASN R 15 | 7 45.112 | -20.618 | -14.145 | 1.00 84.20 | R | Ĉ |
| 10 | ATOM | 1594 | CB ASN R 15 | 7 44.314 | -21.852 | -13.723 | 1.00 84.00 | R | C |
| | ATOM | 1595 | C ASN R 15 O ASN R 15 | | -19.634 -19.808 | | 1.00 82.50 1.00 82.32 | R R | C |
| | MOTA MOTA | 1596 1597 | O ASN R 15 N TYR R 15 | | -18.554 | | 1.00 79.53 | R | N |
| | MOTA | 1598 | CA TYR R 15 | | -17.413 | | 1.00 77.43 | R | C |
| 15 | MOTA | 1599 | CB TYR R 15 | | | -12.968 -14.214 | 1.00 76.44 1.00 75.20 | R R | C |
| | ATOM ATOM | 1600 1601 | CG TYR R 15 CD1 TYR R 15 | | | -15.442 | 1.00 74.38 | R | С |
| | ATOM | 1602 | CE1 TYR R 1 | 8 45.492 | | -16.622 | 1.00 74.67 | R | C |
| 20 | ATOM | 1603 1604 | CD2 TYR R 15 CE2 TYR R 15 | | | -14.174 -15.356 | 1.00 75.41 1.00 75.52 | R R | C |
| 20 | ATOM ATOM | 1604 | CZ TYR R 1 | | -16.109 | -16.571 | 1.00 75.14 | R | č |
| | MOTA | 1606 | OH TYR R 1 | 8 47.584 | | -17.752 | 1.00 76.43 | R | 0 |
| | ATOM | 1607 1608 | C TYR R 15 | | -17.356 -17.732 | -10.910 -10.921 | 1.00 75.97 1.00 75.96 | R R | C |
| 25 | ATOM ATOM | 1609 | N THR R 1 | 9 44.406 | -16.859 | -9.850 | 1.00 74.64 | R | N |
| | ATOM | 1610 | CA THR R 1 | | -16.313 | -8.746 | 1.00 73.18 | R | C |
| | MOTA MOTA | 1611 1612 | CB THR R 1! OG1 THR R 1! | | | -7.471 -7.690 | 1.00 73.25 1.00 73.03 | R R | C O |
| | MOTA | 1613 | CG2 THR R 1 | | | -6.329 | 1.00 72.72 | R | C |
| 30 | MOTA | 1614 | C THR R 1 | • | | -8.503 | 1.00 71.48 | R R | C |
| | MOTA MOTA | 1615 1616 | O THR R 1 | _ | -14.475 -14.036 | -8.413 -8.456 | 1.00 71.07 1.00 69.18 | R R | N |
| | ATOM | 1617 | CA LEU R 1 | | -12.640 | -8.082 | 1.00 67.26 | R | C |
| | ATOM | 1618 | CB LEU R 1 | | | -8.887 -8.500 | 1.00 66.01 1.00 63.77 | R R | C |
| 35 | MOTA MOTA | 1619 1620 | CG LEU R 1 | | | -9.625 | 1.00 63.77 | R | C |
| | MOTA | 1621 | CD2 LEU R 1 | 50 41.328 | -9.945 | -7.286 | 1.00 61.91 | R | C |
| | ATOM | 1622 | C LEUR 1 | | | -6.590 -6.047 | 1.00 66.34 1.00 65.01 | R R | C |
| 40 | ATOM ATOM | 1623 1624 | O LEUR 1 N TYR R 1 | | | -5.927 | 1.00 66.57 | R | N |
| | MOTA | 1625 | CA TYR R 1 | 43.678 | | -4.522 | 1.00 66.28 | R | C |
| | MOTA | 1626 1627 | CB TYR R 1 CG TYR R 1 | | -11.973 -13.444 | -3.713 -3.882 | 1.00 66.76 1.00 68.38 | R R | C |
| | ATOM ATOM | 1628 | CD1 TYR R 1 | | -13.864 | -4.886 | 1.00 68.35 | R | С |
| 45 | ATOM | 1629 | CE1 TYR R 1 | | -15.212 | -5.022 | 1.00 69.74 | R | C |
| | MOTA MOTA | 1630 1631 | CD2 TYR R 1 CE2 TYR R 1 | | -14.394 -15.739 | -2.979 -3.120 | 1.00 69.17 1.00 69.18 | R R | C |
| | ATOM | 1632 | CZ TYR R 1 | | | -4.154 | 1.00 69.89 | R | C |
| | ATOM | 1633 | OH TYR R 1 | 51 46.083 | | -4.369 | 1.00 70.29 | R | 0 |
| 50 | ATOM ATOM | 1634 1635 | C TYR R 1 O TYR R 1 | | | -4.413 -5.258 | 1.00 65.45 1.00 64.16 | R R | С 0 |
| | ATOM | 1636 | N TYR R 1 | 52 42.954 | -9.480 | -3.355 | 1.00 64.72 | R | N |
| | ATOM | 1637 | CA TYR R 1 | | | -3.159 -3.938 | 1.00 66.48 1.00 65.27 | R R | C |
| 55 | MOTA MOTA | 1638 1639 | CB TYR R 1 CG TYR R 1 | | | | 1.00 63.27 | R | C |
| 00 | ATOM | 1640 | CD1 TYR R 1 | 52 39.795 | -7.315 | -2.288 | 1.00 61.94 | R | C |
| | ATOM | 1641 | CE1 TYR R 1 CD2 TYR R 1 | | | | 1.00 61.74 1.00 62.34 | R R | C |
| | MOTA MOTA | 1642 1643 | CE2 TYR R 1 | | | | 1.00 60.23 | R | С |
| 60 | MOTA | 1644 | CZ TYR R 1 | 62 37.979 | -8.896 | -2.274 | 1.00 60.10 | R | C |
| | ATOM | 1645 | OH TYR R 1 | | | | 1.00 58.65 1.00 68.03 | R R | C 0 |
| | ATOM ATOM | 1646 1647 | C TYR R 1 O TYR R 1 | | -8.431 | -0.884 | 1.00 67.34 | R | 0 |
| | ATOM | 1648 | N TRP R 1 | 63 43.337 | 7 -6.564 | -1.311 | 1.00 69.63 | R | N |
| 65 | ATOM ATOM | 1649 1650 | CA TRP R 1 CB TRP R 1 | | | | 1.00 71.19 1.00 71.77 | R R | C |
| | ATOM | 1651 | CG TRP R 1 | 63 44.603 | | 2.122 | 1.00 71.55 | R | C |
| | ATOM | 1652 | CD2 TRP R 1 | 63 45.077 | 7 -4.565 | 2.603 | 1.00 71.76 | R | C |
| | MOTA | 1653 | CE2 TRP R 1 | 63 44.873 | 3 -4.558 | 4.011 | 1.00 71.73 | R | С |

| | | | | | | | | _ | ~ |
|------------|--------------|--------------|--------------------------------|------------------|------------------------|-----------------|--------------------------|--------|--------|
| | ATOM | 1654 | CE3 IKL K T02 | 45.624 | -3.452 | 1.985 | 1.00 72.15 1.00 71.65 | R R | C C |
| | ATOM | 1655 | CD1 TRP R 163 | 44.145 | -6.563 | 3.247 4.401 | 1.00 71.03 | R | N |
| | MOTA | | NE1 TRP R 163 | 44.281 45.232 | -5.856 -3.438 | 4.748 | 1.00 72.72 | R | C |
| | MOTA | | CZ2 TRP R 163 CZ3 TRP R 163 | 45.982 | -2.334 | 2.723 | 1.00 72.41 | R | C |
| 5 | ATOM | | CZ3 TRP R 163 CH2 TRP R 163 | 45.778 | -2.329 | 4.115 | 1.00 72.89 | R | C |
| | ATOM ATOM | | C TRP R 163 | 42.820 | -4.677 | 0.156 | 1.00 72.31 | R | C |
| | ATOM | | O TRP R 163 | 43.177 | 3.0-0 | -0.642 | 1.00 72.04 | R R | N O |
| | ATOM | | N HIS R 164 | 41.961 | -4.446 | 1.146 | 1.00 73.99 1.00 76.09 | R | C |
| 10 | ATOM | 1663 | CA HIS R 164 | 41.637 | -3.058 -2.794 | 1.506 1.057 | 1.00 70.05 | R | č |
| | MOTA | | CB HIS R 164 | 40.202 39.841 | -2.794 -1.359 | 1.320 | 1.00 78.45 | R | C |
| | MOTA | | CG HIS R 164 CD2 HIS R 164 | 40.543 | -0.215 | 0.941 | 1.00 78.66 | R | С |
| | ATOM | 1666 | ND1 HIS R 164 | 38.685 | -0.978 | 1.921 | 1.00 78.84 | R | N |
| 4.5 | MOTA | 1667 1668 | CE1 HIS R 164 | 38.691 | 0.369 | 1.887 | 1.00 77.98 | R | C |
| 15 | MOTA MOTA | 1669 | NE2 HIS R 164 | 39.792 | 0.853 | 1.305 | 1.00 78.68 | R | N C |
| | MOTA | 1670 | C HIS R 164 | 41.748 | -2.882 | 3.018 | 1.00 76.77 1.00 77.29 | R R | Ö |
| | MOTA | 1671 | O HIS R 164 | 41.503 | -3.805 | 3.773 3.483 | 1.00 77.29 | R | N |
| | MOTA | 1672 | N ARG R 165 | 42.179 | -1.699 -1.632 | 4.928 | 1.00 77.00 | R | C |
| 20 | MOTA | 1673 | CA ARG R 165 CB ARG R 165 | 42.376 42.925 | -0.263 | 5.317 | 1.00 77.22 | R | С |
| | ATOM | 1674 | | 41.073 | -1.920 | 5.680 | 1.00 80.09 | R | C |
| | MOTA | 1675 1676 | C ARG R 165 O ARG R 165 | 41.038 | -2.137 | 6.877 | 1.00 80.16 | R | 0 |
| | MOTA MOTA | 1677 | N SER R 166 | 39.956 | -1.909 | 4.929 | 1.00 81.21 | R | N C |
| 25 | MOTA | 1678 | CA SER R 166 | 38.685 | -2.195 | 5.589 | 1.00 82.09 1.00 82.11 | R R | C |
| 20 | ATOM | 1679 | CB SER R 166 | 37.532 | -1.790 | 4.665 5.425 | 1.00 82.11 | R | ŏ |
| | MOTA | 1680 | OG SER R 166 | 36.554 38.567 | -1.082 -3.676 | 5.946 | 1.00 83.27 | R | C |
| | MOTA | 1681 | C SER R 166 O SER R 166 | 37.607 | -4.135 | 6.554 | 1.00 83.85 | R | 0 |
| | MOTA | 1682 | 4 CD | 39.580 | -4.444 | 5.517 | 1.00 83.51 | R | N |
| 30 | ATOM ATOM | 1683 1684 | N LEUR 167 CA LEUR 167 | 39.570 | -5.871 | 5.804 | 1.00 83.71 | R | C |
| | ATOM | 1685 | CB LEU R 167 | 39.571 | -6.633 | 4.480 | 1.00 84.23 | R R | C |
| | ATOM | 1686 | CG LEUR 167 | 38.694 | -5.962 | 3.422 | 1.00 84.47 1.00 84.80 | R | C |
| | MOTA | 1687 | CD1 LEU R 167 | 39.283 | -6.081 | 2.015 3.353 | 1.00 85.44 | R | Č |
| 35 | ATOM | 1688 | CD2 LEU R 167 | 37.288 40.770 | -6.558 -6.292 | 6.650 | 1.00 84.08 | R | С |
| | MOTA | 1689 | C LEUR 167 O LEUR 167 | 41.704 | -5.535 | 6.885 | 1.00 84.12 | R | . 0 |
| | MOTA | 1690 1691 | O LEUR 167 N GLUR 168 | 40.699 | -7.540 | 7.146 | 1.00 84.44 | R | N |
| | MOTA MOTA | 1691 | CA GLUR 168 | 41.780 | -8.060 | 7.970 | 1.00 84.36 | R | C |
| 40 | ATOM | 1693 | CB GLU R 168 | 41.167 | -9.007 | 9.000 | 1.00 83.89 | R R | C |
| 40 | ATOM | 1694 | C GLUR 168 | 42.805 | -8.814 | 7.124 | 1.00 84.52 1.00 84.96 | R | ŏ |
| | MOTA | 1695 | O GLU R 168 | 44.001 | | 7.171 6.400 | 1.00 84.09 | R | N |
| | MOTA | 1696 | N LYS R 169 | 42.272 | -10.648 | 5.594 | 1.00 83.45 | R | C |
| | MOTA | 1697 | CA LYS R 169 CB LYS R 169 | 42.898 | | 6.008 | 1.00 83.34 | R | C |
| 45 | MOTA | 1698 1699 | CB LYS R 169 C LYS R 169 | 42.830 | -10.475 | 4.108 | 1.00 82.71 | R | C |
| | MOTA MOTA | 1700 | O LYS R 169 | 41.740 | -10.102 | 3.691 | 1.00 83.06 | R | N |
| | MOTA | 1701 | N ILE R 170 | 43.881 | -10.711 | 3.315 | 1.00 81.31 1.00 80.46 | R R | C |
| | MOTA | 1702 | CA ILE R 170 | 43.701 | -10.725 | 1.882 1.273 | 1.00 79.74 | R | č |
| 5 0 | MOTA | 1703 | CB ILE R 170 | 44.982 | -11.284 -11.438 | -0.252 | 1.00 79.29 | R | C |
| | ATOM | 1704 | CG2 ILE R 170 CG1 ILE R 170 | 46.135 | -10.307 | 1.515 | 1.00 79.81 | R | С |
| | MOTA | 1705 | CG1 ILE R 170 CD1 ILE R 170 | 47.446 | -11.014 | 1.859 | | R | C |
| | ATOM ATOM | 1706 1707 | C ILE R 170 | 42.504 | 1 -11.587 | 1.506 | | R | C |
| 55 | MOTA | 1708 | | 42.231 | L -12.629 | 2.089 | | R R | N O |
| 30 | ATOM | 1709 | N HIS R 171 | 41.736 | -11.076 | 0.529 | | R | Ĉ |
| | MOTA | 1710 | CA HIS R 171 | 40.563 | L -11.808 | 0.038 -0.014 | | R | č |
| | ATOM | 1711 | | 39.3/3 | 3 -10.829 4 -10.796 | 1.332 | | R | С |
| | MOTA | | CG HIS R 171 | 30.004 | 7 - 11.354 | | | R | С |
| 60 | MOTA | | | 39.17 | 5 -10.114 | 2.395 | 1.00 81.10 | R | N |
| | MOTA | | | 38.26 | 0 -10.249 | 3.376 | | R | C |
| | MOTA MOTA | | | 37.21 | 5 -10.986 | 2.991 | | R | N |
| | ATOM | | C HIS R 171 | 40.79 | 3 -12.475 | -1.345 | | R R | C |
| 65 | ATOM | | 8 O HIS R 171 | 41.75 | 2 - 12.194 | -2.063 | | R | N |
| | ATOM | 1719 | | 39.89 | 1 -13.443 9 -14.228 | -1.669 -2.91 | | R | Ċ |
| | ATOM | | | 39.33 30.70 | 9 -14.226 9 -15.694 | -2.481 | L 1.00 85.66 | R | C |
| | MOTA | | | 41.09 | 5 - 16.484 | | | R | С |
| | MOTA | 1722 | CG GLIN IC 1/2 | 203 | | | | | |
| | | | | /111 | | | | | |

| | ATOM | 1723 | CD GLN R 1 | | 8 -17.862 | -1.831 | 1.00 87.26 | R | C |
|----|--------------|----------------|------------------------------|----------------------|--------------------------|--------------------|--------------------------|--------|--------|
| | ATOM ATOM | 1724 1725 | OE1 GLN R 1' NE2 GLN R 1' | | | -2.282 -0.781 | 1.00 86.59 1.00 86.84 | R R | N O |
| _ | ATOM | 1726 | C GLN R 1 | | | -3.826 | 1.00 85.75 | R | C |
| 5 | ATOM ATOM | 1727 1728 | O GLN R 1' N CYS R 1' | | | -3.434 -5.085 | 1.00 86.57 1.00 87.06 | R R | N O |
| | ATOM | 1729 | CA CYS R 1 | 3 37.94 | 17 -13.228 | -6.011 | 1.00 88.58 | R | C |
| | ATOM ATOM | 1730 1731 | C CYS R 1' O CYS R 1' | | | -6.734 -7.055 | 1.00 89.45 1.00 89.20 | R R | C O |
| 10 | ATOM | 1731 | CB CYS R 1 | | | -7.026 | 1.00 88.12 | R | č |
| | MOTA | 1733 | SG CYS R 1 | | | -8.320 | 1.00 88.29 | R | S |
| | MOTA MOTA | 1734 1735 | N GLUR 1'CA GLUR 1' | | | -6.935 -7.092 | 1.00 91.09 1.00 93.06 | R R | C N |
| | ATOM | 1736 | CB GLU R 1 | 4 35.51 | L5 -16.4 76 | -5.655 | 1.00 92.78 | R | C |
| 15 | ATOM | 1737 | C GLUR 1 | | 94 -16.121 | -7.778 | 1.00 94.86 | R | C |
| | ATOM ATOM | 1738 1739 | O GLUR 1' N ASNR 1' | | | -7.070 -9.167 | 1.00 95.21 1.00 96.51 | R R | N O |
| | MOTA | 1740 | CA ASN R 1 | 5 34.64 | 19 -15.056 | -10.196 | 1.00 98.10 | R | С |
| 20 | MOTA MOTA | $1741 \\ 1742$ | CB ASN R 1' CG ASN R 1' | | 02 -13.645 L9 -13.789 | -10.052 -9.833 | 1.00 97.69 1.00 98.11 | R R | C |
| 20 | ATOM | 1743 | OD1 ASN R 1 | | $\frac{13.763}{11}$ | | 1.00 98.85 | R | ŏ |
| | MOTA | 1744 | ND2 ASN R 1 | | 23 -13.187 | -8.731 | 1.00 97.61 | R | N |
| | MOTA MOTA | 1745 1746 | C ASN R 1'O ASN R 1' | | 94 -15.623 93 -16.274 | | 1.00 98.91 1.00 99.60 | R R | C |
| 25 | MOTA | 1747 | N ILE R 1 | 6 35.93 | 35 -15.304 | -12.313 | 1.00 99.69 | R | N |
| | ATOM | 1748 1749 | CA ILE R 1'CB ILE R 1' | | | | 1.00100.40 1.00101.08 | R R | C |
| | ATOM ATOM | 1750 | CG2 ILE R 1 | | | | 1.00101.79 | R | С |
| | MOTA | 1751 | CG1 ILE R 1 | | | | 1.00100.88 | R | C |
| 30 | ATOM ATOM | 1752 1753 | CD1 ILE R 1 | | | | 1.00101.03 | R R | C C |
| | ATOM | 1754 | O ILE R 1 | 6 38.47 | 71 -15.481 | -14.194 | 1.00100.09 | R | 0 |
| | ATOM | 1755 | N PHE R 1 | | | | 1.00100.98 | R R | N |
| 35 | ATOM ATOM | 1756 1757 | CA PHE R 1 CB PHE R 1 | | | | 1.00101.31 | R R | C |
| • | MOTA | 1758 | CG PHE R 1 | 7 34.89 | 96 -12.665 | -16.040 | 1.00103.06 | R | С |
| | ATOM ATOM | 1759 1760 | CD1 PHE R 1 CD2 PHE R 1 | | | | 1.00103.48 1.00103.36 | R R | C |
| | ATOM | 1761 | CE1 PHE R 1 | | | | 1.00103.30 | R | С |
| 40 | ATOM | 1762 | CE2 PHE R 1 | | | | 1.00103.34 | R | C |
| | ATOM ATOM | 1763 1764 | CZ PHE R 1 C PHE R 1 | | | | 1.00103.07 1.00101.05 | R R | C |
| | ATOM | 1765 | O PHE R 1 | 77 34.6 | 70 -14.993 | -18.554 | 1.00100.84 | R | 0 |
| 45 | MOTA | 1766 1767 | N ARG R 1 CA ARG R 1 | | | | 1.00101.03 1.00101.14 | R R | N C |
| 45 | ATOM ATOM | 1768 | CB ARG R 1 | | | | 1.00101.04 | R | С |
| | ATOM | 1769 | CG ARG R 1 | | 51 -15.629 | | 1.00101.47 | R | C |
| | ATOM ATOM | 1770 1771 | CD ARG R 1 NE ARG R 1 | | 45 -16.797 83 -17.951 | | 1.00102.67 1.00104.10 | R R | C N |
| 50 | MOTA | 1772 | CZ ARG R 1 | 78 38.99 | 91 -18.243 | -23.433 | 1.00104.33 | R | C |
| | MOTA | 1773 1774 | NH1 ARG R 1 NH2 ARG R 1 | | 21 -18.048 99 -18.428 | | 1.00104.55 1.00104.03 | R R | N N |
| | ATOM ATOM | 1775 | C ARG R 1 | | 51 -13.580 | | 1.00101.18 | R | Č |
| | MOTA | 1776 | O ARG R 1 | | 70 -13.903 | | 1.00101.57 | R | 0 |
| 55 | ATOM ATOM | 1777 1778 | N GLUR1 CA GLUR1 | 79 36.6. 79 35.7' | 38 -12.501 73 -11.734 | -21.117 | 1.00100.71 1.00100.14 | R R | N C |
| | ATOM | 1779 | CB GLU R 1 | 79 35.4 | 05 -10.413 | -21.330 | 1.00100.45 | R | C |
| | ATOM | 1780 | CG GLU R 1 | | 99 -10.453 | | 1.00100.59 | R R | C |
| 60 | ATOM ATOM | 1781 1782 | CD GLU R 1 OE1 GLU R 1 | | | -20.073 -19.891 | 1.00100.07 | R R | 0 |
| 00 | ATOM | 1783 | OE2 GLU R 1 | 79 32.5 | 12 -8.909 | -19.746 | 1.00 99.84 | R | 0 |
| | ATOM | 1784 | C GLUR1 | | 55 -11.453 33 -10.331 | -23.353 | 1.00 99.72 1.00 99.74 | R R | C C |
| | ATOM ATOM | 1785 1786 | O GLUR1 N GLYR1 | | 92 -12.538 | | 1.00 98.92 | R | N |
| 65 | ATOM | 1787 | CA GLY R 1 | 37.4 | 21 -12.461 | -25.343 | 1.00 97.33 | R | C |
| | ATOM ATOM | 1788 1789 | C GLY R 1 O GLY R 1 | | 12 -13.017 87 -14.171 | | 1.00 96.44 1.00 96.81 | R R | C |
| | ATOM | 1790 | N GLN R 1 | 39.8 | 18 -12.151 | -25.221 | 1.00 95.64 | R | N |
| | ATOM | 1791 | CA GLN R 1 | 31 41.1 | 90 -12.569 | -24.929 | 1.00 94.60 | R | С |

| | ATOM ATOM ATOM | 1792 1793 1794 | CB GLN R 181 CG GLN R 181 CD GLN R 181 | 42.135 -11.897 -25.932 1.00 93.48 43.453 -12.656 -26.116 1.00 91.79 44.435 -11.767 -26.849 1.00 91.05 | R C R C | 3 |
|----|--------------------------------------|--------------------------------------|--|---|-------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM | 1795 1796 1797 1798 | OE1 GLN R 181 NE2 GLN R 181 C GLN R 181 O GLN R 181 | 45.600 -12.075 -27.043 1.00 90.47 43.907 -10.593 -27.251 1.00 91.76 41.594 -12.197 -23.501 1.00 94.47 42.564 -12.693 -22.947 1.00 94.04 40.835 -11.252 -22.922 1.00 93.91 | | N. |
| 10 | ATOM ATOM ATOM ATOM ATOM | 1799 1800 1801 1802 1803 | N TYR R 182 CA TYR R 182 CB TYR R 182 CG TYR R 182 CD1 TYR R 182 | 41.114 -10.850 -21.550 1.00 92.81 40.414 -9.515 -21.292 1.00 93.02 40.892 -8.460 -22.224 1.00 92.82 39.960 -7.756 -22.982 1.00 92.48 | R C R C R C | 0 0 0 |
| 15 | ATOM ATOM ATOM | 1804 1805 1806 | CE1 TYR R 182 CD2 TYR R 182 CE2 TYR R 182 | 40.309 -6.563 -23.595 1.00 92.44 42.199 -7.976 -22.127 1.00 93.13 42.553 -6.787 -22.749 1.00 92.71 | R (| с С |
| 13 | ATOM ATOM ATOM | 1807 1808 1809 | CZ TYR R 182 OH TYR R 182 C TYR R 182 | 41.613 -6.079 -23.476 1.00 92.01 41.935 -4.857 -24.029 1.00 91.15 40.586 -11.879 -20.547 1.00 92.26 | R (| С О С |
| 20 | ATOM ATOM ATOM ATOM | 1810 1811 1812 1813 | O TYR R 182 N PHE R 183 CA PHE R 183 CB PHE R 183 | 39.683 -12.660 -20.826 1.00 92.36 41.217 -11.890 -19.356 1.00 91.37 40.649 -12.619 -18.222 1.00 90.25 41.700 -13.609 -17.704 1.00 90.91 | R I R C | O N C C |
| 25 | ATOM ATOM ATOM | 1814 1815 1816 | CG PHE R 183 CD1 PHE R 183 CD2 PHE R 183 | 41.817 -14.796 -18.620 1.00 91.41 42.561 -14.689 -19.789 1.00 91.78 41.313 -16.027 -18.226 1.00 91.12 | R (| с с с |
| | MOTA MOTA MOTA | 1817 1818 1819 | CE1 PHE R 183 CE2 PHE R 183 CZ PHE R 183 | 42.812 -15.822 -20.556 | R R | 000 |
| 30 | ATOM ATOM ATOM ATOM | 1820 1821 1822 1823 | C PHE R 183 O PHE R 183 N GLY R 184 CA GLY R 184 | 40.918 -10.596 -16.931 1.00 88.98 39.199 -11.934 -16.373 1.00 87.72 38.721 -10.948 -15.388 1.00 86.34 | R R R | C N O |
| 35 | MOTA MOTA MOTA | 1824 1825 1826 | C GLY R 184 O GLY R 184 N CYS R 185 | 38.097 -11.592 -14.131 1.00 85.86 38.003 -12.806 -14.001 1.00 86.34 37.690 -10.718 -13.175 1.00 85.14 37.169 -11.211 -11.888 1.00 83.61 | R R | 0 N C |
| | ATOM ATOM ATOM | 1827 1828 1829 | CA CYS R 185 C CYS R 185 O CYS R 185 CB CYS R 185 | 37.169 -11.211 -11.888 1.00 83.61 36.513 -10.091 -11.058 1.00 81.56 37.072 -9.024 -10.855 1.00 81.30 38.351 -11.784 -11.104 1.00 85.14 | R R | 000 |
| 40 | ATOM ATOM ATOM ATOM | 1830 1831 1832 1833 | CB CYS R 185 SG CYS R 185 N SER R 186 CA SER R 186 | 37.842 -12.999 -9.871 1.00 89.00 35.267 -10.349 -10.589 1.00 78.90 34.553 -9.318 -9.830 1.00 76.87 | R R R | S N C |
| 45 | ATOM ATOM ATOM | 1834 1835 1836 | CB SER R 186 OG SER R 186 C SER R 186 | 33.162 -9.134 -10.442 1.00 75.93 33.288 -8.740 -11.808 1.00 75.39 34.414 -9.655 -8.338 1.00 76.01 34.220 -10.797 -7.939 1.00 77.16 | R R | 0000 |
| | ATOM ATOM ATOM | 1837 1838 1839 1840 | O SER R 186 N PHE R 187 CA PHE R 187 CB PHE R 187 | 34.220 -10.797 -7.939 1.00 77.16 $34.558 -8.610 -7.499 1.00 74.92$ $34.277 -8.787 -6.077 1.00 74.79$ $35.596 -9.010 -5.328 1.00 73.25$ | R R | C C |
| 50 | ATOM ATOM ATOM ATOM | 1841 1842 1843 | CG PHE R 187 CD1 PHE R 187 CD2 PHE R 187 | 36.588 -7.932 -5.661 1.00 72.03 37.503 -8.143 -6.686 1.00 70.77 36.720 -6.833 -4.825 1.00 71.76 | R R | 000 |
| 55 | MOTA MOTA MOTA MOTA | 1844 1845 1846 1847 | CE1 PHE R 187 CE2 PHE R 187 CZ PHE R 187 C PHE R 187 | 38.562 -7.262 -6.861 1.00 70.31 37.785 -5.952 -5.009 1.00 70.79 38.709 -6.164 -6.023 1.00 70.25 33.533 -7.590 -5.486 1.00 75.47 | R R R R | ממממ |
| | ATOM ATOM ATOM | 1848 1849 1850 | O PHE R 187 N ASP R 188 CA ASP R 188 | 33.632 -6.461 -5.948 1.00 75.75 32.732 -7.881 -4.446 1.00 76.38 31.943 -6.820 -3.832 1.00 77.29 | R R R | ОИС |
| 60 | MOTA MOTA MOTA | 1851 1852 1853 1854 | CB ASP R 188 CG ASP R 188 OD1 ASP R 188 OD2 ASP R 188 | 30.992 -7.454 -2.819 1.00 77.97 29.933 -8.252 -3.559 1.00 79.71 29.265 -9.057 -2.910 1.00 79.83 29.792 -8.069 -4.765 1.00 80.40 | R R R R | 0 0 0 |
| 65 | ATOM ATOM ATOM | 1855 1856 1857 | C ASP R 188 O ASP R 188 N LEU R 189 | 32.812 -5.775 -3.137 1.00 78.25 33.707 -6.088 -2.352 1.00 77.98 32.531 -4.502 -3.479 1.00 79.81 33.321 -3.580 -2.691 1.00 81.28 | R R R R | О И С |
| | ATOM ATOM ATOM | 1858 1859 1860 | CB LEU R 189 | 34.356 -2.914 -3.632 1.00 79.95 35.761 -2.840 -3.015 1.00 78.56 | R R | C |

| | I | 75 648 _1 751 _3.654 1.00 77.86 | R C |
|----|--|--|-------------|
| | ATOM 1861 CD1 LEU R 189 | 36.646 -1.731 -1.516 1.00 78.01 | R C |
| | ATOM 1862 CD2 LEU R 189 | 33.742 2.541 -2.088 1.00 83.89 | R C |
| | 711011 D 100 | 32.422 -1.413 -2.462 1.00 85.14 | R O R N |
| 5 | ATOM 1865 N THR R 190 | 31.455 -5.001 - 756 1 00 80 32 | R C |
| 3 | ATOM 1866 CA THR R 190 | 30.489 -2.231 0.767 1.00 90.54 | R C |
| | ATOM 1867 CB THR R 190 ATOM 1868 OG1 THR R 190 | 28.694 -3.084 -2.088 1.00 92.85 | R O R C |
| | ATOM 1868 OG1 THR R 190 ATOM 1869 CG2 THR R 190 | 28.164 -1.538 -0.343 1.00 90.98 | R C |
| 10 | ATOM 1870 C THR R 190 | 30.043 4.00 1 00 00 03 | r O |
| 10 | ATOM 1871 O THR R 190 | 30.407 -0.782 0.535 1.00 91.79 | R N |
| | ATOM CAR TAKE B 101 | 30.894 0.095 1.314 1.00 92.71 | R C R C |
| | ATOM 1874 CB LYS R 191 | 32.426 -0.031 1.665 1.00 92.75 33.388 -0.275 0.516 1.00 93.39 | R C |
| 15 | ATOM 1875 CG LYS R 191 | 33.300 0.27 1 00 04 00 | R C |
| .0 | ATOM 1876 CD LYS R 191 | 24.659 -0.069 2.504 1.00 94.65 | R C |
| | H1011 101 | 36.364 0.035 2.909 1.00 95.24 | R N R C |
| | ATOM 1879 C LYS R 191 | 30.462 1.359 0.829 1.00 93.00 | R O |
| 20 | ATOM 1880 O LYS R 191 | 30.002 1.001 1.873 1.00 93.44 | R N |
| | ATOM 1881 N VAL R 192 ATOM 1882 CA VAL R 192 | 21 280 2 942 2 087 1.00 93.53 | R C |
| | 111011 1000 CD 173T D 102 | 31.435 3.571 0.713 1.00 93.72 | R· C R C |
| | ATOM 1884 CG1 VAL R 192 | 30.322 4.534 0.286 1.00 92.98 32.731 4.246 0.833 1.00 93.28 | R C |
| 25 | ATOM 1885 CG2 VAL R 192 | 30.690 3.764 3.176 1.00 93.63 | R C |
| | ATOM 1886 C VAL R 192 ATOM 1887 O VAL R 192 | 29.651 3.300 3.700 1.00 93.63 | R O R N |
| | ATOM 1887 O VAL R 192 ATOM 1888 N SER R 195 | 34.830 5.067 5.044 1.00 93.32 | R N R C |
| | ATTOM 1889 CA SER R 195 | 33.300 3.62 7 141 1 00 92 62 | R C |
| 30 | ATOM 1890 CB SER R 195 | 37 171 6 115 5.185 1.00 92.89 | R C |
| | ATOM 1891 C SER R 195 ATOM 1892 O SER R 195 | 37.818 7.054 5.590 1.00 92.98 | R O R N |
| | ATOM 1893 N SER R 196 | 37.582 5.349 4.160 1.00 92.61 | R C |
| | ATOM 1894 CA SER R 196 | 38.282 5.902 3.006 1.00 92.21 39.563 6.681 3.449 1.00 92.18 | R C |
| 35 | ATOM 1895 CB SER R 196 | 38.603 4.704 2.105 1.00 92.05 | R C |
| | ATOM 1896 C SER R 196 ATOM 1897 O SER R 196 | 38.832 3.608 2.597 1.00 91.91 | R O R N |
| | ATOM 1898 N PHE R 197 | 38.653 4.865 0.787 1.00 91.69 38.379 6.028 0.271 1.00 89.94 | R C |
| | ATOM 1899 CA PHE R 197 | 39.573 6.751 -0.864 1.00 89.28 | R C |
| 40 | ATOM 1900 CB PHE R 197 | 40.855 5.709 0.058 1.00 89.62 | R C |
| | A1011 2302 | 41.507 6.163 -0.868 1.00 89.86 | R O R N |
| | ATOM 1903 N PHE R 198 | 41.500 2.500 2.501 1.00 87 68 | R C |
| | ATOM 1904 CA PHE R 198 | 42.333 3.415 2.196 1.00 88.99 | R C |
| 45 | ATOM 1905 CB PHE R 198 | 42.938 4.418 3.273 1.00 90.06 | R C R C |
| | ATOM 1906 CG PHE R 198 ATOM 1907 CD1 PHE R 198 | 42.004 4.407 4.300 1.00 90.80 | R C |
| | ATTOM 1908 CD2 PHE R 198 | 44.000 0000 - 000 1 00 01 06 | R C |
| | ATOM 1909 CE1 PHE R 198 | 44 105 6 111 4.405 1.00 90.95 | R C |
| 50 | ATOM 1910 CE2 PHE R 198 ATOM 1911 CZ PHE R 198 | 43.260 6.120 5.439 1.00 91.49 | R C R C |
| | 7TOM 1912 C PHE R 198 | 42.231 2.909 -0.085 1.00 86.57 41.270 2.156 0.109 1.00 86.67 | R O |
| | ATOM 1913 O PHE R 198 | 41.270 2.156 0.109 1.00 86.67 43.093 2.726 -1.119 1.00 84.73 | R N |
| | ATOM 1914 N GLU R 199 | 42 683 1.886 -2.249 1.00 82.61 | R C R C |
| 55 | ALULA CT T D 100 | 43.575 2.234 -3.415 1.00 83.35 | R C R C |
| | ATOM 1917 CG GLU R 199 | 40.040 | R C |
| | ATOM 1918 CD GLU R 199 | 46 028 3 143 -2.922 1.00 91.39 | R O |
| | ATOM 1919 OE1 GLU R 199 ATOM 1920 OE2 GLU R 199 | 45.020 4.943 -4.082 1.00 88.27 | R O |
| 60 | A1011 - 0111 D 100 | 42.773 0.369 -1.990 1.00 79.66 | R C R O |
| | ATOM 1922 O GLU R 199 | 43.549 -0.104 -1.171 1.00 80.10 | R N |
| | ATOM 1923 N GLN R 200 | 42 204 -1 807 -2 879 1.00 75.22 | R C |
| | ATOM 1924 CA GLN R 200 | 41.174 -2.437 -3.820 1.00 74.17 | R C |
| 65 | 222 D 200 | 43.612 -1.900 -3.458 1.00 73.89 | R C R O |
| | ATTOM 1927 O GLN R 200 | 43.967 -1.288 -4.445 1.00 73.99 44.285 -2.810 -2.734 1.00 72.01 | R N |
| | ATOM 1928 N HIS R 201 | 44.285 -2.810 -2.734 1.00 72.01 45.391 -3.514 -3.381 1.00 69.70 | R C |
| | ATOM 1929 CA HIS R 201 | 43.334 0.0 | |
| | | 206 | |

| | | | | 46 851 -3.159 -3.012 1.00 72.07 | R (| С |
|-----|--------------|-------------------|-------------------------------|--|--------|--------|
| | MOTA | 1930 CE | | 46.851 -3.159 -3.012 1.00 72.07 47.274 -3.528 -1.597 1.00 74.38 | | C |
| | MOTA | 1931 CG | | 46.774 -2.989 -0.388 1.00 75.58 | | C |
| | ATOM | | 02 HIS R 201 01 HIS R 201 | 48 592 -3.870 -1.379 1.00 75.68 | | N |
| _ | MOTA MOTA | | E1 HIS R 201 | 48 907 -3.380 -0.174 1.00 75.89 | | C |
| 5 | MOTA | 1935 NE | E2 HIS R 201 | 47.848 -2.827 0.437 1.00 76.65 | | N |
| | MOTA | 1936 C | HIS R 201 | 45.003 -4.779 -4.170 1.00 67.12 44.002 -5.417 -3.872 1.00 65.87 | | С О |
| | MOTA | 1937 O | HIS R 201 | ==.002 1 00 CE 76 | | N |
| | MOTA | 1938 N | SER R 202 | 45.751 -5.050 -5.270 1.00 65.76 45.327 -6.188 -6.091 1.00 65.49 | | C |
| 10 | ATOM | 1939 CZ | | 44.495 -5.649 -7.263 1.00 65.59 | | С |
| | ATOM | 1940 CF | | 43.098 -5.779 -6.969 1.00 66.07 | | 0 |
| | MOTA | 1941 OC 1942 C | | 46 535 -6.973 -6.619 1.00 65.89 | | C |
| | ATOM ATOM | 1942 C | | 47.599 -6.431 -6.871 1.00 64.15 | | 0 |
| 15 | MOTA | 1944 N | | 46.327 -8.302 -6.744 1.00 66.75 | | N C |
| 10 | ATOM | 1945 C | A GLN R 203 | 47.399 -9.168 -7.251 1.00 67.38 48.204 -9.679 -6.053 1.00 66.69 | R | C |
| | MOTA | 1946 C | | 10.20 | | Č |
| | MOTA | 1947 C | | 46.855 -10.371 -8.053 1.00 68.36 45.854 -10.977 -7.702 1.00 66.91 | R | Ō |
| | MOTA | 1948 O | | 47.509 -10.732 -9.173 1.00 70.11 | R | N |
| 20 | MOTA | 1949 N 1950 C | | 47.017 -11.891 -9.892 1.00 72.85 | R | C |
| | MOTA MOTA | 1951 C | | 46.510 -11.420 -11.254 1.00 71.76 | R | C |
| | MOTA | 1952 C | | 48.130 -12.914 -10.099 1.00 74.05 | R R | C O |
| | ATOM | 1953 O | ILE R 204 | 49.095 -12.693 -10.811 1.00 73.69 47.999 -14.052 -9.402 1.00 75.96 | R | N |
| 25 | ATOM | 1954 N | | 47.333 | R | C |
| | MOTA | | A MET R 205 | 48.967 -15.105 -9.673 1.00 78.62 49.965 -15.225 -8.509 1.00 79.44 | R | C |
| | MOTA | | B MET R 205 G MET R 205 | 49 402 -15.843 -7.222 1.00 81.81 | R | C |
| | MOTA MOTA | | G MET R 205 D MET R 205 | 50.703 -16.108 -6.007 1.00 82.92 | R | S |
| 30 | MOTA | | E MET R 205 | 49.674 -16.308 -4.546 1.00 82.58 | R | C |
| 50 | ATOM | 1960 C | MET R 205 | 48.319 -16.438 -10.013 1.00 79.83 47 111 -16.605 -10.058 1.00 79.06 | R R | 0 |
| | ATOM | 1961 C | | 47.111 | R | N |
| | MOTA | 1962 N | VAL R 206 | 49.208 -17.383 -10.328 1.00 81.92 48.799 -18.755 -10.495 1.00 84.18 | R | C |
| | MOTA | | CA VAL R 206 CB VAL R 206 | 49.721 -19.384 -11.537 1.00 84.11 | R | C |
| 35 | MOTA | 1964 C | CB VAL R 206 CG1 VAL R 206 | 49.508 -18.739 -12.903 1.00 84.53 | R | C |
| | MOTA MOTA | 1966 | CG2 VAL R 206 | 51.157 -19.192 -11.105 1.00 84.63 | R | C |
| | ATOM | | C VAL R 206 | 48.967 -19.544 -9.205 1.00 85.81 | R R | C |
| | ATOM | | O VAL R 206 | 49.967 -19.462 -8.501 1.00 85.71 47.908 -20.307 -8.873 1.00 87.72 | R | N |
| 40 | MOTA | | N LYS R 207 | =7.500 = 5.00 00 00 | R | C |
| | MOTA | | CA LYS R 207 CB LYS R 207 | 48.237 -21.691 -8.645 1.00 89.82 46.928 -22.445 -8.381 1.00 88.83 | R | C |
| | MOTA | | CB LYS R 207 CG LYS R 207 | 45.916 -21.599 -7.591 1.00 87.18 | R | C |
| | MOTA MOTA | | CD LYS R 207 | 44 806 -21.024 -8.473 1.00 84.32 | R. | C |
| 45 | ATOM | | CE LYS R 207 | 43.626 -21.989 -8.659 1.00 83.21 | R R | C N |
| 0 | ATOM | | NZ LYS R 207 | 42.370 -21.243 -8.795 1.00 81.54 48.838 -22.108 -9.996 1.00 91.87 | R | C |
| | MOTA | | C LYS R 207 | 48.838 -22.108 -9.996 1.00 91.87 48.713 -21.364 -10.971 1.00 92.75 | R | Ō |
| | MOTA | | O LYS R 207 N ASP R 208 | 49.540 -23.245 -10.062 1.00 93.36 | R | N |
| EO | MOTA MOTA | | N ASP R 208 CA ASP R 208 | 49 966 -24.006 -8.913 1.00 94.52 | R | C |
| 50 | ATOM | | CB ASP R 208 | 49.743 -25.487 -9.287 1.00 95.14 | R | C |
| | ATOM | 1981 | CG ASP R 208 | 50.314 -26.476 -8.267 1.00 94.52 50.551 -26.079 -7.124 1.00 95.08 | R R | Ö |
| | MOTA | 1982 | OD1 ASP R 208 | 30.332 | R | ŏ |
| | MOTA | | OD2 ASP R 208 | 50.425 -27.653 -8.606 1.00 94.46 51.439 -23.684 -8.693 1.00 95.30 | R | Č |
| 55 | MOTA | _ | C ASP R 208 O ASP R 208 | 52.313 -24.168 -9.392 1.00 95.25 | R | 0 |
| | MOTA | | 000 | 51.688 -22.736 -7.775 1.00 95.46 | R | N |
| | MOTA MOTA | | N ASN R 209 CA ASN R 209 | 53.074 -22.593 -7.285 1.00 95.80 | R | C |
| | MOTA | 1988 | CB ASN R 209 | 53.647 -23.981 -6.970 1.00 95.91 | R | C |
| 60 | MOTA | 1989 | C ASN R 209 | 53.914 -21.882 -8.310 1.00 95.80 | R R | 0 |
| | MOTA | 1990 | O ASN R 209 | 55.114 -21.672 -8.150 1.00 96.45 53.272 -21.535 -9.471 1.00 94.72 | R | И |
| | MOTA | | N ALA R 210 | 53.272 -21.535 -9.471 1.00 94.72 53.984 -20.679 -10.372 1.00 94.16 | R | Ĉ |
| | MOTA | | CA ALA R 210 | 55.324 -20.490 -9.802 1.00 93.34 | R | С |
| 0.5 | MOTA | | CB ALA R 210 C ALA R 210 | 54.173 -21.188 -11.727 1.00 94.18 | R | C |
| 65 | MOTA | | O ALA R 210 | 54.019 -22.340 -12.136 1.00 94.20 | R | 0 |
| | ATOM ATOM | | N GLY R 211 | 54.350 -20.070 -12.407 1.00 94.38 | R R | С И |
| | MOTA | | CA GLY R 211 | 55.687 -19.730 -12.616 1.00 94.63 55.979 -18.821 -13.853 1.00 95.21 | R R | C |
| | MOTA | | C GLY R 211 | | | |
| | | | | 207 | | |

| | ATOM | 1999 | 0 | GLY R | 211 | 57.147 | -18.479 | -14.185 | 1.00 96.27 | | R | 0 |
|-----|------|------|-------------|-------|-----|--------|---------|---------|------------|---|---|-------------|
| | | 2000 | | LYS R | | | -18.419 | | | | | |
| | ATOM | | N | | | | | | 1.00 94.97 | | R | N |
| | MOTA | 2001 | CA | LYS R | | 53.509 | -18.475 | -14.380 | 1.00 94.25 | | R | C |
| | ATOM | 2002 | CB | LYS R | 212 | 52.637 | -18.475 | -15.650 | 1.00 94.92 | * | R | C |
| 5 | ATOM | 2003 | C | LYS R | | 53.083 | | -13.420 | 1.00 93.59 | | R | Č |
| 9 | | | | | | | | | | | | |
| | MOTA | 2004 | 0 | LYS R | | | | | 1.00 93.83 | | R | 0 |
| | ATOM | 2005 | N | ILE R | 213 | 53.894 | -17.246 | -12.371 | 1.00 92.42 | | R | N |
| | ATOM | 2006 | CA | ILE R | 213 | 54.088 | -15.920 | -11.881 | 1.00 91.16 | | R | C |
| | | | | | | | | | | | | |
| | MOTA | 2007 | CB | ILE R | | | -16.057 | | 1.00 91.36 | | R | C |
| 10 | ATOM | 2008 | C | ILE R | 213 | 55.216 | -15.382 | -12.781 | 1.00 90.27 | | R | C |
| | MOTA | 2009 | 0 | ILÉ R | 213 | 55 931 | -16.146 | -13 391 | 1.00 91.19 | | R | 0 |
| | | | | | | | | | | | | |
| | ATOM | 2010 | N | LYS R | | 55.449 | | -12.885 | 1.00 88.61 | | R | N |
| | ATOM | 2011 | ca | LYS R | 214 | 55.517 | -13.243 | -11.735 | 1.00 86.29 | | R | C |
| | ATOM | 2012 | CB | LYS R | 214 | 56.288 | -12.003 | -12.189 | 1.00 86.22 | | R | C |
| 4.5 | | | | | | | | | | | | ă |
| 15 | MOTA | 2013 | С | LYS R | | 54.163 | | -11.268 | 1.00 84.26 | | R | С |
| | ATOM | 2014 | 0 | LYS R | 214 | 53.269 | -12.542 | -12.049 | 1.00 84.28 | | R | 0 |
| | ATOM | 2015 | N | PRO R | 215 | 53.988 | -12.879 | 9.968 | 1.00 81.59 | | R | N |
| | | | | PRO R | | | | -8.962 | | | | |
| | ATOM | 2016 | CD | | | 54.698 | | | 1.00 80.19 | | R | C |
| | MOTA | 2017 | ca | PRO R | 215 | 52.980 | | -9.392 | 1.00 79.54 | | R | С |
| 20 | ATOM | 2018 | CB | PRO R | 215 | 53.302 | -11.929 | -7.903 | 1.00 80.09 | | R | C |
| | ATOM | 2019 | CG | PRO R | | 54.360 | | -7.554 | 1.00 80.43 | | R | Ċ |
| | | | | | | | | | | | | _ |
| | MOTA | 2020 | C | PRO R | | 53.026 | | | 1.00 77.50 | | R | С |
| | ATOM | 2021 | 0 | PRO R | 215 | 54.099 | -10.107 | -10.259 | 1.00 77.69 | | R | 0 |
| | ATOM | 2022 | N | SER R | | 51.828 | | -10.616 | 1.00 75.99 | | R | N |
| 0.5 | | | | | | | | | | | | |
| 25 | ATOM | 2023 | ca | SER R | | 51.660 | | -11.042 | 1.00 74.40 | | R | С |
| | ATOM | 2024 | CB | SER R | 216 | 51.054 | -8.795 | -12.451 | 1.00 74.52 | | R | C |
| | ATOM | 2025 | OG | SER R | 216 | 51.361 | | -13.070 | 1.00 75.58 | | R | 0 |
| | | | | | | | | | | | | |
| | MOTA | 2026 | С | SER R | | 50.712 | -8.058 | -10.081 | 1.00 73.20 | | R | С |
| | ATOM | 2027 | 0 | SER R | 216 | 49.594 | -8.459 | -9.784 | 1.00 72.12 | | R | 0 |
| 30 | MOTA | 2028 | N | PHE R | 217 | 51.253 | -6.957 | -9.506 | 1.00 72.00 | | R | N |
| •• | ATOM | 2029 | | PHE R | | 50.463 | -6.155 | -8.580 | 1.00 71.16 | | R | |
| | | | CA | | | | | | | | | C |
| | ATOM | 2030 | CB | PHE R | 217 | 51.351 | -5.718 | -7.410 | 1.00 71.05 | | R | C |
| | MOTA | 2031 | CG | PHE R | 217 | 52.005 | -6.881 | -6.740 | 1.00 71.64 | | R | С |
| | ATOM | 2032 | | PHE R | | 53.247 | -7.331 | -7.192 | 1.00 72.43 | | R | Č |
| | | | | | | | | | | | | ~ |
| 35 | MOTA | 2033 | CD2 | PHE R | 217 | 51.379 | -7.498 | -5.662 | 1.00 71.96 | | R | ,C |
| | MOTA | 2034 | CE1 | PHE R | 217 | 53.872 | -8.369 | -6.543 | 1.00 71.92 | | R | С |
| | ATOM | 2035 | CE2 | | | 52.024 | | -5.008 | 1.00 72.65 | | R | Ċ |
| | | | | | | | | | | | | ~ |
| | ATOM | 2036 | CZ | PHE R | 217 | 53.284 | | -5.431 | 1.00 72.45 | | R | С |
| | MOTA | 2037 | С | PHE R | 217 | 49.876 | -4.897 | -9.226 | 1.00 69.71 | | R | C |
| 40 | ATOM | 2038 | ō | PHE R | | 50.434 | | -10.167 | 1.00 69.81 | | R | ŏ |
| 40 | | | | | | | | | | | | |
| | MOTA | 2039 | N | ASN R | | 48.709 | | -8.796 | 1.00 69.22 | | R | N |
| | ATOM | 2040 | $^{\rm CA}$ | ASN R | 218 | 48.378 | -3.039 | -9.002 | 1.00 67.82 | | R | С |
| | MOTA | 2041 | CB | ASN R | 218 | 47.499 | | -10.262 | 1.00 68.56 | | R | С |
| | | | | | | | | | | | | |
| | MOTA | 2042 | CG | ASN R | | 47.411 | | -11.083 | 1.00 69.14 | | R | C |
| 45 | MOTA | 2043 | OD1 | ASN R | 218 | 46.282 | -1.290 | -11.316 | 1.00 68.24 | | R | 0 |
| | MOTA | 2044 | ND2 | ASN R | 218 | 48.550 | -1.234 | -11.638 | 1.00 69.11 | | R | N |
| | | 2045 | C | | | 47.685 | | | 1.00 67.04 | | R | ĉ |
| | MOTA | | | ASN R | | | | -7.829 | | | | |
| | MOTA | 2046 | 0 | ASN R | | 46.882 | | -7.054 | 1.00 67.27 | | R | 0 |
| | MOTA | 2047 | N | ILE R | 219 | 47.882 | -1.008 | -7.739 | 1.00 65.28 | | R | N |
| 50 | ATOM | 2048 | CA | ILE R | | 47.072 | | -6.782 | 1.00 62.22 | | R | C |
| 50 | | | | | | | | | | | | \tilde{a} |
| | MOTA | 2049 | CB | ILE R | | 47.889 | | -6.154 | 1.00 61.26 | | R | С |
| | MOTA | 2050 | CG2 | ILE R | 219 | 47.089 | 1.423 | -5.015 | 1.00 60.00 | | R | С |
| | ATOM | 2051 | CG1 | | | 49.245 | | -5.849 | 1.00 60.74 | | R | C |
| | | | | | | | | | | | | ă |
| | MOTA | 2052 | CD1 | | | 49.142 | | -4.532 | 1.00 61.59 | | R | C |
| 55 | MOTA | 2053 | С | ILE R | 219 | 45.912 | 0.453 | -7.427 | 1.00 60.80 | | R | C |
| | MOTA | 2054 | 0 | ILE R | 219 | 46.063 | 1.318 | -8.100 | 1.00 60.85 | | R | 0 |
| | | 2055 | | VAL R | | 44.725 | | -6.972 | 1.00 59.05 | | | |
| | ATOM | | N | | | | | | | | R | N |
| | MOTA | 2056 | ca | VAL R | | 43.615 | | -7.625 | 1.00 58.49 | | R | С |
| | MOTA | 2057 | CB | VAL R | 220 | 42.595 | -0.222 | -7.732 | 1.00 58.24 | | R | С |
| 60 | ATOM | 2058 | | VAL R | | 41.264 | | -7.943 | 1.00 57.03 | | R | Č |
| 00 | | | | | | | | | | | | ~ |
| | MOTA | 2059 | | VAL R | | 42.879 | | -8.784 | 1.00 58.45 | | R | С |
| | MOTA | 2060 | C | VAL R | 220 | 43.046 | 1.823 | -6.630 | 1.00 59.18 | | R | С |
| | ATOM | 2061 | Ō | VAL R | | 42.640 | | -5.576 | 1.00 58.01 | | R | Ō |
| | | | | | | | | | | | | |
| | MOTA | 2062 | N | PRO R | | 43.019 | | -6.931 | 1.00 59.22 | | R | N |
| 65 | MOTA | 2063 | $^{\rm CD}$ | PRO R | 221 | 43.756 | 3.682 | -8.065 | 1.00 59.51 | | R | С |
| | MOTA | 2064 | CA | PRO R | | 42.377 | | -6.016 | 1.00 59.09 | | R | С |
| | MOTA | 2065 | CB | PRO R | | 43.035 | | -6.332 | 1.00 59.17 | | R | Ċ |
| | | | | | | | | | | | | ۲ |
| | MOTA | 2066 | CG | PRO R | | 43.602 | | -7.714 | 1.00 60.65 | | R | С |
| | ATOM | 2067 | С | PRO R | 221 | 40.916 | 4.053 | -6.228 | 1.00 58.55 | | R | С |
| | | | | | | | | | | | | |

| | ATOM | 2068 | 0 | PRO R 2 | 221 | 40.365 | 3.642 | -7.271 | 1.00 5 | 57.97 | R | 0 |
|----|--------------|----------------|------------|---------|-----|------------------|----------------|--------------------|--------|----------------|--------|--------------|
| | ATOM | 2069 | N | LEU R 2 | | 40.307 | 4.324 | -5.110 | | 8.65 | R | N |
| | MOTA | 2070 | CA | LEU R 2 | | 38.862 | 4.396 | -4.976 | | 59.43 | R | С |
| _ | MOTA | 2071 | CB | LEU R 2 | | 38.401 | 3.880 | -3.581 | | 59.09 | R | C |
| 5 | ATOM | 2072 2073 | CG | LEU R 2 | | 38.866 38.159 | 2.400 | -3.381 -2.020 | | 59.86 59.90 | R R | C |
| | ATOM ATOM | 2073 | | LEU R 2 | | 38.159 | 2.093 1.312 | -2.020 -4.282 | | 59.54 | R R | C |
| | ATOM | 2075 | C | LEU R 2 | | 38.335 | 5.826 | -5.198 | | 59.51 | R | Č |
| | ATOM | 2076 | ō | LEU R 2 | | 37.141 | 6.194 | -4.797 | | 50.14 | R | Ō |
| 10 | MOTA | 2077 | N | THR R 2 | | 39.177 | 6.628 | -5.887 | | 59.04 | R | N |
| | ATOM | 2078 | CA | THR R 2 | | 38.769 | 8.017 | -6.126 | 1.00 6 | | R | C |
| | ATOM | 2079 | CB OC1 | THR R 2 | | 39.803 41.112 | 8.955 8.701 | -5.469 -6.077 | 1.006 | 58.81 | R | C |
| | MOTA MOTA | 2080 2081 | OG1 CG2 | THR R 2 | | 39.943 | 8.602 | -3.942 | 1.00 5 | | R R | С О |
| 15 | MOTA | 2082 | C | THR R 2 | | 38.586 | 8.352 | -7.661 | | 51.12 | R | č |
| | ATOM | 2083 | ō | THR R 2 | | 38.600 | 9.585 | -7.991 | 1.00 6 | | R | Ō |
| | MOTA | 2084 | N | SER R 2 | | 38.761 | 7.327 | -8.481 | | 50.44 | R | N |
| | ATOM | 2085 | CA | SER R 2 | | 38.631 | 7.431 | -9.949 | | 50.05 | R | C |
| 20 | ATOM ATOM | 2086 2087 | CB OG | SER R 2 | | 39.940 40.975 | | -10.698 -10.323 | 1.00 5 | 59.15 | R R | C |
| 20 | ATOM | 2087 | C | SER R 2 | | 38.190 | | -10.509 | 1.00 | | R | C |
| | ATOM | 2089 | ŏ | SER R 2 | | 37.994 | 5.195 | -9.813 | | 50.32 | R | ō |
| | MOTA | 2090 | N | ARG R 2 | | 37.989 | | -11.805 | 1.00 | 50.24 | R | N |
| | MOTA | 2091 | CA | ARG R | | 37.473 | | -12.554 | | 50.06 | R | С |
| 25 | ATOM | 2092 | CB | ARG R | | 38.651 | | -12.686 | 1.00 | | R | C |
| | ATOM ATOM | 2093 2094 | CG CD | ARG R 2 | | 39.769 41.050 | | -13.915 -13.667 | | 52.36 54.74 | R R | C |
| | ATOM | 2095 | NE | ARG R | | 40.782 | | -14.166 | | 58.21 | R | N |
| | ATOM | 2096 | CZ | ARG R 2 | | 40.836 | | -15.433 | | 59.76 | R | C |
| 30 | ATOM | 2097 | NH1 | | | 41.215 | | -16.406 | 1.00 | | R | N |
| | ATOM | 2098 | NH2 | | | 40.462 | | -15.754 | | 58.97 | R | Ŋ |
| | MOTA | 2099 | C | ARG R | | 36.261 36.180 | | -11.811 -11.400 | 1.00 | 58.98 58.24 | R R | C |
| | ATOM ATOM | $2100 \\ 2101$ | N O | ARG R 2 | | 35.242 | | -11.400 | 1.00 5 | | R R | NO |
| 35 | MOTA | 2102 | CA | VAL R | | 33.963 | | -11.138 | | 57.67 | R | C |
| | ATOM | 2103 | CB | VAL R | | 33.581 | 5.553 | -9.962 | | 57.05 | R | Č |
| | ATOM | 2104 | | VAL R | | 32.230 | 5.098 | -9.412 | 1.00 5 | | R | С |
| | ATOM | 2105 | | VAL R | | 34.626 | 5.400 | -9.019 | | 56.30 | R | C |
| 40 | MOTA | 2106 | C | VAL R 2 | | 32.929 32.683 | | -12.171 -12.594 | 1.00 5 | 57.20 57.69 | R R | C |
| 40 | ATOM ATOM | 2107 2108 | N O | LYS R | | 32.277 | | -12.432 | 1.00 | | R | И |
| | ATOM | 2109 | CA | LYS R | | 31.173 | | -13.343 | | 55.34 | R | Ĉ |
| | MOTA | 2110 | CB | LYS R | | 31.412 | 2.625 | -14.480 | | 56.41 | R | C |
| | MOTA | 2111 | CG | LYS R 2 | | 30.200 | | -15.576 | | 58.70 | R | С |
| 45 | ATOM | 2112 | CD | LYS R | | 30.323 | | -16.396 | | 50.42 | R | C |
| | ATOM ATOM | 2113 2114 | CE NZ | LYS R | | 29.315 29.788 | | -17.612 -18.509 | 1.00 (| | R R | C N |
| | ATOM | 2115 | C | LYS R | | 29.725 | | -12.754 | 1.00 | | R | C |
| | ATOM | 2116 | ŏ | LYS R | | 29.399 | | -12.202 | 1.00 ! | | R | ŏ |
| 50 | MOTA | 2117 | N | PRO R | 228 | 28.953 | | -12.738 | 1.00 5 | | R | N |
| | ATOM | 2118 | CD | PRO R | | 29.263 | | -13.221 | 1.00 5 | | R | C |
| | MOTA | $2119 \\ 2120$ | CA | PRO R | | 27.716 27.255 | | -12.075 -12.135 | 1.00 5 | | R R | C |
| | ATOM ATOM | 2121 | CB CG | PRO R : | | 28.408 | | -12.135 -12.531 | 1.00 ! | | R | C |
| 55 | ATOM | 2122 | C | PRO R | | 26.782 | | -12.908 | 1.00 | | R | Č |
| | ATOM | 2123 | 0 | PRO R | | 26.949 | 3.618 | -14.112 | 1.00 5 | | R | 0 |
| | MOTA | 2124 | N | ASP R | | 25.778 | | -12.223 | 1.00 | | R | \mathbf{N} |
| | ATOM | 2125 | CA | ASP R | | 24.575 | | -12.833 | 1.00 5 | | R | C |
| 60 | ATOM ATOM | 2126 2127 | CB CG | ASP R | | 23.619 23.773 | | -11.626 -11.364 | 1.00 ! | | R R | C |
| 00 | ATOM | 2128 | | ASP R | | 22.857 | | -11.364 -10.684 | 1.00 | | R | 0 |
| | ATOM | 2129 | OD2 | ASP R | 229 | 24.745 | | -11.874 | 1.00 | | R | ŏ |
| | MOTA | 2130 | C | ASP R | | 23.875 | | -13.620 | 1.00 | | R | C |
| | MOTA | 2131 | 0 | ASP R | 229 | 24.155 | | -13.521 | 1.00 9 | | R | 0 |
| 65 | ATOM | 2132 | N | PRO R | | 22.902 | | -14.361 | 1.00 5 | | R | N |
| | MOTA | $2133 \\ 2134$ | CD | PRO R | | 22.655 22.149 | | -14.865 -15.096 | 1.00 ! | | R R | C |
| | MOTA MOTA | 2134 | CA CB | PRO R | | 21.618 | | -16.264 | 1.00 | | R | C |
| | ATOM | 2136 | CG | PRO R | | 21.439 | | -15.823 | 1.00 | | R | Č |
| | | | | | | | | | | | | |

| | | | | | | | _ | ~ |
|-----|--------------|----------------|-------------------------------|------------------|----------------------------------|--------------------------|--------|---|
| | MOTA | 2137 | C PRO R 230 | 21.032 | 5.316 -14.361 | 1.00 50.11 | R | C |
| | MOTA | 2138 | O PRO R 230 | 20.585 | 4.913 -13.309 | 1.00 49.02 | R | 0 |
| | MOTA | 2139 | N PRO R 231 | 20.645 | 6.470 -14.824 | 1.00 49.41 | R | N |
| | MOTA | 2140 | CD PRO R 231 | 21.209 | 7.201 -15.948 | 1.00 47.62 1.00 49.23 | R R | C |
| 5 | MOTA | 2141 | CA PRO R 231 | 19.558 | 7.155 -14.158 | 1.00 49.23 | R | C |
| | MOTA | 2142 | CB PRO R 231 | 19.820 | 8.559 -14.487 | 1.00 48.87 | R | C |
| | MOTA | 2143 | CG PRO R 231 | 20.363 | 8.402 -15.906 | 1.00 50.36 | R | Č |
| | MOTA | 2144 | C PRO R 231 | 18.225 | 6.726 -14.621 5.913 -15.535 | 1.00 30.30 | R | ŏ |
| | ATOM | 2145 | O PRO R 231 | 18.108 | 7.294 -14.050 | 1.00 51.65 | R | N |
| 10 | ATOM | 2146 | N HIS R 232 | 17.184 | 6.777 -14.461 | 1.00 55.01 | R | Ĉ |
| | ATOM | 2147 | CA HIS R 232 | 15.898 15.326 | 5.916 -13.298 | 1.00 58.75 | R | Č |
| | ATOM | 2148 | CB HIS R 232 CG HIS R 232 | 16.040 | 4.570 -13.111 | 1.00 64.23 | R | Ċ |
| | MOTA | 2149 | CG HIS R 232 CD2 HIS R 232 | 17.226 | 4.301 -12.418 | 1.00 66.01 | R | Č |
| 4.5 | MOTA | 2150 | ND1 HIS R 232 | 15.509 | 3.378 -13.508 | 1.00 66.21 | R | N |
| 15 | ATOM | $2151 \\ 2152$ | CE1 HIS R 232 | 16.394 | 2.428 -13.135 | 1.00 66.33 | R | C |
| | MOTA | 2152 | NE2 HIS R 232 | 17.424 | 2.951 -12.477 | 1.00 67.23 | R | N |
| | ATOM ATOM | 2154 | C HIS R 232 | 14.984 | 7.987 -14.716 | 1.00 54.86 | R | С |
| | ATOM | 2155 | O HIS R 232 | 14.789 | 8.823 -13.855 | 1.00 55.11 | R | 0 |
| 20 | ATOM | 2156 | N ILE R 233 | 14.490 | 8.130 -15.957 | 1.00 55.90 | R | N |
| 20 | ATOM | 2157 | CA ILE R 233 | 13.668 | 9.309 -16.230 | 1.00 57.90 | R | С |
| | ATOM | 2158 | CB ILE R 233 | 13.488 | 9.425 -17.746 | 1.00 55.99 | R | С |
| | ATOM | 2159 | CG2 ILE R 233 | 12.523 | 10.592 -18.052 | 1.00 54.70 | R | С |
| | ATOM | 2160 | CG1 ILE R 233 | 14.820 | 9.768 -18.450 | 1.00 54.05 | R | С |
| 25 | ATOM | 2161 | CD1 ILE R 233 | 14.821 | 9.352 -19.932 | 1.00 51.18 | R | C |
| | ATOM | 2162 | C ILE R 233 | 12.296 | 9.207 -15.516 | 1.00 59.58 | R | C |
| | ATOM | 2163 | O ILE R 233 | 11.658 | 8.168 -15.524 | 1.00 60.77 | R | 0 |
| | ATOM | 2164 | N LYS R 234 | 11.885 | 10.306 -14.815 | 1.00 62.94 | R | N |
| | MOTA | 2165 | CA LYS R 234 | 10.553 | 10.308 - 14.137 | 1.00 66.66 | R | C |
| 30 | MOTA | 2166 | CB LYS R 234 | 10.612 | 11.067 -12.787 | 1.00 67.92 | R | C |
| | MOTA | 2167 | CG LYS R 234 | 11.368 | 10.348 -11.657 | 1.00 71.28 | R | C |
| | MOTA | 2168 | CD LYS R 234 | 11.312 | 11.168 -10.373 | 1.00 73.35 | R | C |
| | MOTA | 2169 | CE LYS R 234 | 11.778 | 10.430 -9.129 | 1.00 75.77 | R R | И |
| | MOTA | 2170 | NZ LYS R 234 | 12.379 | 11.410 -8.240 | 1.00 77.02 | R R | C |
| 35 | MOTA | 2171 | C LYS R 234 | 9.421 | 10.914 -15.004 | 1.00 68.02 1.00 68.12 | R | o |
| | MOTA | 2172 | O LYS R 234 | 8.393 | 10.292 -15.238 | 1.00 69.38 | R | И |
| | MOTA | 2173 | N ASN R 235 | 9.597 | 12.200 -15.425 | 1.00 09.38 | R | Ĉ |
| | MOTA | 2174 | CA ASN R 235 | 8.652 | 12.746 -16.405 13.438 -15.735 | 1.00 72.11 | R | Č |
| | ATOM | 2175 | CB ASN R 235 | 7.476 | 13.450 -16.725 | 1.00 75.24 | R | č |
| 40 | ATOM | 2176 | CG ASN R 235 | 6.324 5.944 | 12.424 -17.277 | 1.00 77.18 | R | ŏ |
| | ATOM | 2177 | OD1 ASN R 235 | | 14.635 -16.867 | 1.00 75.83 | R | N |
| | ATOM | 2178 | ND2 ASN R 235 C ASN R 235 | | 13.669 -17.448 | 1.00 72.52 | R | ĉ |
| | MOTA | 2179 | | | 14.173 -17.321 | 1.00 73.58 | R | 0 |
| 45 | ATOM ATOM | 2180 2181 | O ASN R 235 N LEU R 236 | | 13.806 -18.543 | 1.00 72.32 | R | N |
| 45 | ATOM | 2182 | CA LEU R 236 | | 14.830 -19.552 | 1.00 72.18 | R | C |
| | ATOM | 2183 | CB LEU R 236 | | 14.173 -20.879 | 1.00 71.35 | R | С |
| | ATOM | 2184 | CG LEU R 236 | | 13.126 -20.782 | 1.00 70.86 | R | C |
| | ATOM | 2185 | CD1 LEU R 236 | | 12.196 -21.988 | 1.00 69.29 | R | С |
| 50 | ATOM | 2186 | CD2 LEU R 236 | | 13.777 -20.782 | 1.00 70.35 | R | C |
| 00 | ATOM | 2187 | C LEU R 236 | | 15.666 -19.730 | 1.00 72.55 | R | C |
| | MOTA | 2188 | O LEU R 236 | | 15.210 -19.575 | 1.00 72.54 | R | 0 |
| | ATOM | 2189 | N SER R 237 | 7.699 | 16.922 -20.088 | 1.00 72.99 | R | N |
| | ATOM | 2190 | CA SER R 237 | 6.545 | 17.784 -20.314 | 1.00 74.18 | R | C |
| 55 | ATOM | 2191 | CB SER R 237 | | 18.006 -18.979 | 1.00 72.83 | R | C |
| | MOTA | 2192 | OG SER R 237 | | 18.620 -18.060 | 1.00 72.56 | R | 0 |
| | MOTA | 2193 | C SER R 237 | | 19.125 -20.925 | 1.00 76.06 | R | C |
| | MOTA | 2194 | O SER R 23 | 8.116 | 19.510 -20.949 | 1.00 76.03 | R | 0 |
| | MOTA | 2195 | N PHE R 238 | 5.936 | 19.820 -21.477 | 1.00 77.57 | R | й |
| 60 | MOTA | 2196 | CA PHE R 238 | | 21.066 -22.176 | 1.00 79.64 | R | C |
| | ATOM | 2197 | CB PHE R 238 | 5.311 | 21.142 -23.399 | 1.00 77.79 | R | C |
| | ATOM | 2198 | CG PHE R 23 | 5.618 | 20.018 -24.344 | 1.00 76.60 | R | C |
| | MOTA | 2199 | CD1 PHE R 23 | 4.694 | 18.993 -24.509 | 1.00 75.57 | R | C |
| | MOTA | 2200 | CD2 PHE R 23 | | 20.072 -25.139 | 1.00 76.20 | R | C |
| 65 | MOTA | 2201 | CE1 PHE R 23 | | 18.029 -25.485 | 1.00 74.70 | R | C |
| | MOTA | 2202 | CE2 PHE R 23 | | 19.100 -26.117 | 1.00 75.82 | R | C |
| | MOTA | 2203 | CZ PHE R 23 | | 18.079 -26.297 | 1.00 75.62 | R | C |
| | MOTA | 2204 | C PHE R 23 | | | | R | C |
| | MOTA | 2205 | O PHE R 23 | 5.041 | 22.374 -20.523 | 1.00 82.54 | R | J |

| | ATOM | 2206 | N HIS R 2 | | 6.933 [,] | 23.247 -21.387 | 1.00 84.05 | R | N |
|-----|--------------|----------------------|----------------------------|------|--------------------|----------------------------------|--------------------------|--------|--------|
| | ATOM ATOM | 2207 2208 | CA HIS R 2 CB HIS R 2 | | 6.730 7.562 | 24.522 -20.723 24.539 -19.451 | 1.00 86.76 1.00 88.55 | R R | C |
| 2 | MOTA | 2209 | CG HIS R 2 | | 8.087 | 25.935 -19.238 | 1.00 90.57 | R | С |
| 5 | MOTA | 2210 | CD2 HIS R 2 | | 9.335 | 26.327 -18.739 | 1.00 91.49 | R | C |
| | MOTA | $2211 \\ 2212$ | ND1 HIS R 2 CE1 HIS R 2 | | 7.373 8.164 | 27.051 -19.528 28.090 -19.201 | 1.00 91.70 1.00 92.58 | R R | C N |
| | MOTA ATOM | 2213 | NE2 HIS R 2 | | 9.347 | 27.689 -18.726 | 1.00 92.38 | R | N |
| | ATOM | 2214 | C HIS R 2 | | 7.180 | 25.668 -21.621 | 1.00 87.52 | R | C |
| 10 | ATOM | 2215 | O HIS R 2 | | 8.347 | 25.994 -21.715 | 1.00 87.44 | R | 0 |
| | MOTA ATOM | 2216 2217 | N ASN R 2 CA ASN R 2 | | 6.204 6.572 | 26.256 -22.310 27.235 -23.314 | 1.00 88.29 1.00 88.24 | R R | С И |
| | ATOM | 2218 | CB ASN R | | 7.705 | 28.079 -22.739 | 1.00 88.25 | R | Č |
| | MOTA | 2219 | C ASN R 2 | 240 | 7.026 | 26.486 -24.568 | 1.00 88.02 | R | С |
| 15 | ATOM | 2220 | O ASN R | | 6.444 | 25.488 -24.980 | 1.00 88.51 | R | O M |
| | MOTA ATOM | 2221 2222 | N ASP R 2 CA ASP R 2 | | 8.086 8.400 | 26.970 -25.210 26.251 -26.430 | 1.00 87.16 1.00 86.30 | R R | N C |
| | ATOM | 2223 | CB ASP R | | 8.645 | 27.275 -27.532 | 1.00 87.95 | R | C |
| 40 | ATOM | 2224 | CG ASP R | | 7.339 | 28.063 -27.722 | 1.00 87.67 | R | C |
| 20 | ATOM ATOM | 2225 2226 | OD1 ASP R 2 | | 6.295 7.367 | 27.510 -27.353 29.216 -28.150 | 1.00 88.15 1.00 88.12 | R R | 0 |
| | ATOM | 2227 | C ASP R | | 9.531 | 25.218 -26.253 | 1.00 85.04 | R | Č |
| | MOTA | 2228 | O ASP R | | 10.205 | 24.828 -27.191 | 1.00 85.17 | R | 0 |
| 0.5 | MOTA | 2229 2230 | N ASPR | | 9.583 | 24.714 -25.000 23.872 -24.616 | 1.00 82.57 1.00 80.06 | R R | N |
| 25 | ATOM ATOM | 2231 | CA ASP R CB ASP R | | 10.706 11.390 | 24.580 -23.455 | 1.00 80.08 | R | C |
| | MOTA | 2232 | CG ASP R | | 12.185 | 25.775 -23.943 | 1.00 81.48 | R | Ċ |
| | MOTA | 2233 | OD1 ASP R | | 12.368 | 25.864 -25.151 | 1.00 81.91 | R | 0 |
| 30 | ATOM ATOM | 223 <u>4</u> 2235 | OD2 ASP R C | | 12.603 10.272 | 26.595 -23.124 22.492 -24.112 | 1.00 81.63 1.00 78.44 | R R | 0 |
| 30 | MOTA | 2236 | O ASP R | | 9.123 | 22.088 -24.167 | 1.00 79.46 | R | Ö |
| | MOTA | 2237 | N LEUR | 243 | 11.276 | 21.763 -23.574 | 1.00 75.69 | R | N |
| | ATOM | 2238 | CA LEU R | | 11.000 | 20.446 -23.006 19.394 -24.018 | 1.00 73.52 1.00 72.84 | R R | G G |
| 35 | MOTA MOTA | 2239 2240 | CB LEU R C | | 11.458 10.788 | 18.034 -23.804 | 1.00 72.09 | R | C |
| 00 | ATOM | 2241 | CD1 LEU R | | 11.612 | 16.882 -24.382 | 1.00 71.29 | R | C |
| | MOTA | 2242 | CD2 LEU R | | 10.574 | 17.709 -22.327 | 1.00 72.11 | R | C |
| | ATOM ATOM | 2243 2244 | C LEUR C | | 11.741 12.963 | 20.241 -21.680 20.186 -21.631 | 1.00 72.81 1.00 73.08 | R R | C |
| 40 | ATOM | 2245 | N TYR R | | 10.928 | 20.170 -20.611 | 1.00 71.27 | R | N |
| | MOTA | 2246 | CA TYR R | | 11.479 | 19.957 -19.278 | 1.00 70.19 | R | C |
| | MOTA | 2247 | CB TYR R CG TYR R | | $10.477 \\ 11.149$ | 20.516 -18.267 20.761 -16.963 | 1.00 72.06 1.00 74.30 | R R | G G |
| | MOTA MOTA | 2248 2249 | CG TYR R CD1 TYR R | | 12.307 | 21.534 -16.907 | 1.00 74.30 | R | C |
| 45 | ATOM | 2250 | CE1 TYR R | 244 | 12.891 | 21.829 -15.679 | 1.00 76.01 | R | C |
| | ATOM | 2251 | CD2 TYR R | | 10.590 | 20.273 -15.782 | 1.00 75.12 | R | C |
| | ATOM ATOM | 2252 2253 | CE2 TYR R CZ TYR R | | 11.178 12.323 | 20.559 -14.558 21.329 -14.503 | 1.00 74.79 1.00 75.92 | R R | C |
| | ATOM | 2254 | OH TYR R | 244 | 12.891 | 21.640 -13.282 | 1.00 75.92 | R | 0 |
| 50 | ATOM | 2255 | C TYR R | | 11.696 | 18.468 -18.999 | 1.00 68.92 | R | C |
| | ATOM ATOM | 2256 2257 | O TYR R N VAL R | | 10.784 12.972 | 17.653 -19.015 18.115 -18.762 | 1.00 67.48 1.00 68.19 | R R | N O |
| | ATOM | 2258 | CA VAL R | | 13.238 | 16.721 -18.435 | 1.00 66.99 | R | Ċ |
| | MOTA | 2259 | CB VAL R | 245 | 14.344 | 16.187 -19.341 | 1.00 67.14 | R | C |
| 55 | ATOM | 2260 | CG1 VAL R CG2 VAL R | | 14.629 13.902 | 14.717 -19.009 16.280 -20.790 | 1.00 65.54 1.00 65.15 | R R | G G |
| | ATOM ATOM | 2261 2262 | C VAL R | | 13.573 | 16.529 -16.954 | 1.00 66.24 | R | Č |
| | ATOM | 2263 | O VAL R | 245 | 14.270 | 17.314 -16.315 | 1.00 66.44 | R | 0 |
| 00 | ATOM | 2264 | N GLN R | | 12.997 | 15.441 -16.403 | 1.00 65.56 | R | И |
| 60 | ATOM ATOM | 2265 2266 | CA GLN R CB GLN R | | 13.115 11.739 | 15.140 -14.975 15.396 -14.333 | 1.00 65.49 1.00 67.51 | R R | C |
| | ATOM | 2267 | CG GLN R | | 11.831 | 15.846 -12.870 | 1.00 70.06 | R | C |
| | ATOM | 2268 | CD GLN R | | 10.691 | 16.796 -12.544 | 1.00 71.11 | R | C |
| 65 | MOTA MOTA | 2269 2270 | OE1 GLN R NE2 GLN R | | 9.698 10.872 | 16.922 -13.247 17.488 -11.400 | 1.00 70.54 1.00 70.86 | R R | N |
| 0.5 | ATOM | 2271 | C GLN R | 246 | 13.551 | 13.684 -14.765 | 1.00 64.64 | R | Ĉ |
| | ATOM | 2272 | O GLN R | | 13.068 | 12.760 -15.412 | 1.00 65.52 | R | 0 |
| | ATOM | 2273 | N TRP R | | 14.536 | 13.493 -13.858 | 1.00 63.78 1.00 62.34 | R R | N C |
| | MOTA | 2274 | CA TRP R | 4± / | 15.092 | 12.144 -13.688 | 1.00 02.34 | K | C |

| | | 16.108 11.890 -14.805 1.00 61.18 | R C |
|----|--|--|------------|
| | ATOM 2275 CB TRP R 247 ATOM 2276 CG TRP R 247 | 17.394 12.599 -14.573 1.00 60.79 | R C R C |
| | ATOM 2277 CD2 TRP R 247 ATOM 2278 CE2 TRP R 247 | 19.140 14.100 -14.767 1.00 60.10 | R C R C |
| 5 | ATOM 2279 CE3 TRP R. 247 | 18.522 12.107 -13.876 1.00 60.74 | R C |
| | ATOM 2281 NE1 TRP R 247 | 19.596 12.942 -13.960 1.00 59.43 19.780 15.266 -15.160 1.00 58.49 | R N R C |
| | ATOM 2282 CZ2 TRP R 247 ATOM 2283 CZ3 TRP R 247 | 17.783 15.957 -16.349 1.00 57.78 | R C R C |
| 10 | ATOM 2284 CH2 TRP R 247 | 15.735 11.884 -12.316 1.00 62.27 | R C |
| | ATOM 2286 O TRP R 247 | 16.012 12.776 -11.535 1.00 61.13 | R O R N |
| | ATOM 2287 N GLU R 248 | 16.487 10.148 -10.767 1.00 64.61 | R C R C |
| 15 | ATOM 2289 CB GLU R 248 | 15.536 9.101 -10.183 1.00 66.82 16.044 8.487 -8.879 1.00 72.44 | R C |
| | ATOM 2290 CG GLU R 248 ATOM 2291 CD GLU R 248 | 15.069 7.423 -8.426 1.00 75.78 | R C R O |
| | ATOM 2292 OE1 GLU R 248 | 14.483 6.766 -9.286 1.00 77.17 | R O R C |
| 20 | ATOM 2294 C GLU R 248 | 17.881 9.547 -10.959 1.00 63.40 18.079 8.578 -11.678 1.00 62.30 | R O |
| | ATOM 2295 O GLU R 248 ATOM 2296 N ASN R 249 | 18.882 10.192 -10.330 1.00 63.16 | R N R C |
| | ATOM 2297 CA ASN R 249 | 21 207 10.669 -9.845 1.00 61.84 | R C |
| 25 | ATOM 2299 CG ASN R 249 | 21.375 11.809 -10.817 1.00 61.58 21.437 11.627 -12.030 1.00 61.61 | R O |
| | ATOM 2300 OD1 ASN R 249 ATOM 2301 ND2 ASN R 249 | 21.469 13.026 -10.253 1.00 61.70 | R N R C |
| | ATOM 2302 C ASN R 249 | 19.469 8.000 -8.814 1.00 63.48 | R O |
| 30 | ATOM 2304 N PRO R 250 | 21.409 7.584 -9.878 1.00 63.57 22.444 7.800 -10.874 1.00 63.27 | R C |
| | ATOM 2305 CD PRO R 250 ATOM 2306 CA PRO R 250 | 21.674 6.361 -9.133 1.00 64.11 | R C R C |
| | ATOM 2307 CB PRO R 250 | 23 260 6 432 -11.023 1.00 63.95 | R C |
| 35 | ATOM 2309 C PRO R 250 | 21.840 6.661 -7.639 1.00 65.15 | R C R O |
| | ATOM 2310 O PRO R 250 ATOM 2311 N GLN R 251 | 21.135 5.861 -6.818 1.00 66.03 | R N R C |
| | ATOM 2312 CA GLN R 251 | 20.367 4.987 -4.687 1.00 69.33 | R C |
| 40 | ATOM 2314 CG GLN R 251 | 19.467 5.423 -3.526 1.00 74.19 | R C R C |
| | ATOM 2315 CD GLN R 251 ATOM 2316 OE1 GLN R 251 | 17.614 4.144 -2.674 1.00 76.89 | R O R N |
| | ATOM 2317 NE2 GLN R 251 | 22 406 6 500 -4.729 1.00 63.78 | R C |
| 45 | ATOM 2319 O GLN R 251 | 22.511 7.392 -3.905 1.00 63.33 | R O R N |
| | ATOM 2320 N ASN R 252 ATOM 2321 CA ASN R 252 | 24.780 5.877 -4.463 1.00 60.52 | R C R C |
| | ATOM 2322 CB ASN R 252 | 25.678 | R C |
| 50 | ATOM 2324 OD1 ASN R 252 | 25.580 2.328 -4.860 1.00 58.57 | R O R N |
| | ATOM 2325 ND2 ASN R 252 ATOM 2326 C ASN R 252 | 25.513 7.161 -4.868 1.00 60.26 | R C R O |
| | ATOM 2327 O ASN R 252 | 26.552 7.522 -4.312 1.00 59.23 25.003 7.814 -5.924 1.00 59.77 | R N |
| 55 | ATOM 2329 CA PHE R 253 | 25.624 9.048 -6.322 1.00 59.18 | R C R C |
| 00 | ATOM 2330 CB PHE R 253 | 26.911 7.957 -8.123 1.00 55.92 | R C R C |
| | ATOM 2332 CD1 PHE R 253 | 26.452 6.655 -8.263 1.00 55.78 28.269 8.256 -8.278 1.00 55.39 | R C |
| 60 | ATOM 2333 CD2 PHE R 253 ATOM 2334 CE1 PHE R 253 | 27.360 5.635 -8.533 1.00 55.18 | R C R C |
| 00 | ATOM 2335 CE2 PHE R 253 | 28.712 5.920 -8.691 1.00 56.84 | R Ċ |
| | ATOM 2337 C PHE R 253 | 24.723 10.189 -6.034 1.00 59.89 23.509 10.088 -5.964 1.00 61.22 | R O |
| 65 | ATOM 2338 O PHE R 253 ATOM 2339 N ILE R 254 | 25.384 11.301 -5.843 1.00 60.15 | R N R C |
| 00 | ATOM 2340 CA ILE R 254 | 25.335 12.928 -4.205 1.00 62.03 | R C |
| | ATOM 2342 CG2 ILE R 254 | 26.791 12.411 -4.197 1.00 63.18 25.389 14.447 -4.172 1.00 62.64 | R C R C |
| | ATOM 2343 CG1 ILE R 254 | 212 | |

| | 7 (110) (| 2244 | CD1 | TT 13 13 25 | = 1 | 26.001 | 14.971 | -2.876 | 1.00 62.24 | R | С |
|----|--------------|--------------|------------|--------------------|-----|------------------|------------------|--------------------|--------------------------|--------|--------|
| | ATOM ATOM | 2344 2345 | CDI | ILE R 25 | | 24.926 | 13.483 | -6.590 | 1.00 59.07 | R | Č |
| | ATOM | 2346 | Õ | ILE R 25 | | 25.969 | 13.482 | -7.255 | 1.00 59.16 | R | 0 |
| | ATOM | 2347 | Ň | SER R 25 | | 23.996 | 14.309 | -6.862 | 1.00 58.74 | R | N |
| 5 | MOTA | 2348 | CA | SER R 25 | | 23.956 | 15.080 | -8.086 | 1.00 58.94 | R | C |
| | MOTA | 2349 | CB | SER R 25 | | 22.644 | 15.831 | -8.045 | 1.00 58.94 | R | C |
| | MOTA | 2350 | OG | SER R 25 | | 22.458 | 16.746 | -9.147 | 1.00 62.51 1.00 58.42 | R R | C |
| | ATOM | 2351 | C | SER R 25 | | 25.122 25.599 | 15.995 16.070 | -8.454 -9.628 | 1.00 58.42 1.00 58.51 | R | Ö |
| 40 | ATOM | 2352 2353 | O N | SER R 25 | | 25.583 | 16.759 | -7.484 | 1.00 57.50 | R | N |
| 10 | ATOM ATOM | 2354 | CA | ARG R 25 | | 26.653 | 17.643 | -7.758 | 1.00 55.75 | R | Ĉ |
| | ATOM | 2355 | CB | ARG R 25 | | 26.808 | 18.702 | -6.582 | 1.00 57.39 | R | C |
| | ATOM | 2356 | CG | ARG R 25 | | 27.236 | 18.154 | -5.258 | 1.00 58.42 | R | С |
| | ATOM | 2357 | CD | ARG R 25 | 56 | 27.694 | 19.178 | -4.274 | 1.00 58.58 | R | C |
| 15 | ATOM | 2358 | NE | ARG R 2 | | 27.686 | 18.482 | -2.990 | 1.00 60.41 | R | N |
| | ATOM | 2359 | CZ | ARG R 2 | | 26.577 | 18.201 | -2.279 | 1.00 60.88 | R R | C N |
| | ATOM | 2360 | NH1 | ARG R 2 | | 25.360 | 18.530 17.611 | -2.655 -1.141 | 1.00 59.81 1.00 60.03 | R | N |
| | ATOM | 2361 2362 | NH2 | ARG R 2 | | 26.693 27.938 | 16.926 | -8.025 | 1.00 53.84 | R | C |
| 20 | MOTA MOTA | 2363 | C C | ARG R 2 | | 28.885 | 17.569 | -8.396 | 1.00 52.44 | R | ŏ |
| 20 | ATOM | 2364 | N | CYS R 2 | | 27.983 | 15.636 | -7.866 | 1.00 52.68 | R | N |
| | ATOM | 2365 | CA | CYS R 2 | | 29.166 | 14.845 | -8.206 | 1.00 52.72 | R | С |
| | ATOM | 2366 | C | CYS R 2 | 57 | 29.178 | 14.290 | -9.641 | 1.00 51.14 | R | C |
| | MOTA | 2367 | 0 | CYS R 2 | 57 | 30.145 | 13.655 | -10.058 | 1.00 50.47 | R | 0 |
| 25 | ATOM | 2368 | CB | CYS R 2 | | 29.186 | 13.673 | -7.249 | 1.00 54.19 | R R | C S |
| | ATOM | 2369 | SG | CYS R 2 | | 29.650 28.143 | 14.132 | -5.568 -10.377 | 1.00 60.74 1.00 48.40 | R | N |
| | ATOM | 2370 2371 | N CA | LEU R 2 | | 27.918 | 13.913 | -11.614 | 1.00 47.82 | R | Ċ |
| | ATOM ATOM | 2372 | CB | LEU R 2 | | 26.655 | | -11.529 | 1.00 46.62 | R | Č |
| 30 | MOTA | 2373 | CG | LEU R 2 | | 26.504 | | -10.673 | 1.00 47.57 | R | C |
| 00 | ATOM | 2374 | | LEU R 2 | | 25.160 | | -10.859 | 1.00 48.25 | R | C |
| | ATOM | 23.75 | CD2 | LEU R 2 | | 27.535 | | -11.209 | 1.00 45.86 | R | C |
| | ATOM | 2376 | С | LEU R 2 | | 27.783 | | -12.653 | 1.00 47.12 | R | C |
| | MOTA | 2377 | 0 | LEU R 2 | | 27.275 | | -12.364 | 1.00 46.63 | R R | N |
| 35 | MOTA | 2378 | N | PHE R 2 | | 28.101 27.739 | 15.318 | -13.826 -15.113 | 1.00 45.55 1.00 45.70 | R | C |
| | MOTA | 2379 2380 | CA CB | PHE R 2 PHE R 2 | | 28.971 | | -15.963 | 1.00 46.66 | R | č |
| | ATOM ATOM | 2381 | CG | PHE R 2 | | 29.726 | 17.012 | | 1.00 49.54 | R | Č |
| | ATOM | 2382 | | PHE R 2 | | 29.244 | 17.725 | -14.274 | 1.00 49.69 | R | C |
| 40 | ATOM | 2383 | CD2 | | | 30.981 | 17.457 | | 1.00 50.86 | R | C |
| | MOTA | 2384 | CE1 | | | 29.902 | | -13.682 | 1.00 50.58 | R | C |
| | MOTA | 2385 | CE2 | | | 31.690 | 18.722 | | 1.00 50.28 | R | C |
| | ATOM | 2386 | CZ | PHE R 2 | | 31.152 | | -14.260 -15.962 | 1.00 50.45 1.00 46.12 | R R | C |
| 45 | MOTA | 2387 | C | PHE R 2 PHE R 2 | | 26.845 26.928 | | -15.914 | 1.00 46.40 | R | ŏ |
| 45 | MOTA MOTA | 2388 2389 | O N | TYR R 2 | | 26.097 | 15.063 | | 1.00 45.23 | R | Ñ |
| | ATOM | 2390 | CA | TYR R 2 | | 25.091 | | -17.606 | 1.00 45.84 | R | C |
| | ATOM | 2391 | CB | TYR R 2 | | 23.650 | 14.675 | -17.082 | 1.00 46.70 | R | С |
| | ATOM | 2392 | CG | TYR R 2 | 60 | 23.579 | | -15.612 | 1.00 49.36 | R | C |
| 50 | MOTA | 2393 | CD1 | | | 23.861 | | -15.000 | 1.00 50.50 | R | C |
| | MOTA | 2394 | CE1 | | | 23.852 | | -13.479 | 1.00 52.78 1.00 49.26 | R R | C |
| | ATOM | 2395 | CD2 | | | 23.241 23.133 | | -14.809 -13.473 | 1.00 49.20 | R | C |
| | ATOM ATOM | 2396 2397 | CE2 CZ | TYR R 2 | | 23.544 | | -12.762 | 1.00 53.08 | R | Č |
| 55 | ATOM | 2398 | OH | TYR R 2 | | 23.422 | | -11.316 | 1.00 56.10 | R | Ō |
| 00 | ATOM | 2399 | C | TYR R 2 | | 25.158 | 14.463 | -19.098 | 1.00 45.82 | R | С |
| | ATOM | 2400 | O | TYR R 2 | 260 | 25.518 | | -19.703 | 1.00 46.96 | R | 0 |
| | ATOM | 2401 | N | GLU R 2 | | 24.649 | | -19.772 | 1.00 45.39 | R | N |
| | MOTA | 2402 | CA | GLU R 2 | | 24.356 | | -21.222 | 1.00 44.70 | R | C |
| 60 | ATOM | 2403 | CB | GLU R 2 | | 25.294 | | -21.907 | 1.00 42.68 1.00 46.04 | R R | C |
| | ATOM | 2404 | CG | GLU R 2 | | 26.123 27.233 | 10 67 <i>6</i> | -22.942 -23.736 | 1.00 48.58 | R | C |
| | MOTA | 2405 2406 | CD OF 1 | GLUR 2 LGLUR 2 | | 28.384 | | -23.750 | 1.00 48.48 | R | ŏ |
| | ATOM ATOM | 2406 | OE | | | 26.918 | | -24.307 | 1.00 50.76 | R | ŏ |
| 65 | ATOM | 2407 | C | GLU R 2 | | 22.852 | 13.311 | -21.527 | 1.00 44.68 | R | C |
| - | ATOM | 2409 | ō | GLU R 2 | | 22.356 | 12.280 | -21.353 | 1.00 44.51 | R | 0 |
| | ATOM | 2410 | N | VAL R 2 | | 22.148 | | -22.026 | 1.00 43.07 | R | И |
| | ATOM | 2411 | CA | VAL R 2 | | 20.816 | | -22.348 | 1.00 44.29 | R | C |
| | ATOM | 2412 | CB | VAL R 2 | 262 | 20.003 | 15.258 | -21.830 | 1.00 43.85 | R | С |

| | MOTA | 2413 | CG1 VAL R 26 | | 15.075 -22.070 | 1.00 43.87 | R | C |
|----|--------------|----------------|-----------------------------|----------|----------------------------------|--------------------------|--------|--------------|
| | MOTA | 2414 | CG2 VAL R 26 | | 15.536 -20.345 | 1.00 43.73 | R | C |
| | MOTA | 2415 | C VAL R 26 | | 14.112 -23.893 | 1.00 45.69 | R | C |
| | MOTA | 2416 | O VAL R 26 | | 15.105 -24.535 | 1.00 45.95 | R | 0 |
| 5 | ATOM | 2417 | N GLU R 26 | | 12.971 -24.382 | 1.00 47.42 | R | N |
| | ATOM | 2418 | CA GLU R 26 | | 12.647 -25.633 | 1.00 49.96 | R | C |
| | ATOM | 2419 | CB GLU R 26 | | 11.119 -25.870 10.749 -27.461 | 1.00 51.56 1.00 53.01 | R R | C |
| | ATOM | 2420 | CG GLU R 26 | | 9.223 -27.656 | 1.00 55.42 | R | C |
| 10 | MOTA | $2421 \\ 2422$ | CD GLU R 26 OE1 GLU R 26 | | 8.628 -28.122 | 1.00 56.59 | R | ŏ |
| 10 | MOTA MOTA | 2423 | OE2 GLU R 26 | | 8.513 -27.239 | 1.00 57.62 | R | ŏ |
| | ATOM | 2424 | C GLU R 26 | | 12.852 -26.019 | 1.00 50.75 | R | č |
| | ATOM | 2425 | O GLU R 26 | | 12.312 -25.460 | 1.00 48.99 | R | Õ |
| | ATOM | 2426 | N VAL R 26 | | 13.621 -27.087 | 1.00 52.50 | R | N |
| 15 | ATOM | 2427 | CA VAL R 26 | | 13.878 -27.641 | 1.00 54.11 | R | C |
| .0 | ATOM | 2428 | CB VAL R 26 | | 15.309 -27.377 | 1.00 53.62 | R | C |
| | ATOM | 2429 | CG1 VAL R 26 | | 15.521 -27.633 | 1.00 51.79 | R | C |
| | ATOM | 2430 | CG2 VAL R 26 | 16.569 | 15.771 -25.785 | 1.00 52.95 | R | C |
| | MOTA | 2431 | C VAL R 26 | | 13.636 -29.117 | 1.00 55.80 | R | Ç |
| 20 | MOTA | 2432 | O VAL R 26 | | 14.292 -29.756 | 1.00 56.07 | R | 0 |
| | MOTA | 2433 | n ASN R 26 | | 12.729 -29.615 | 1.00 58.16 | R | N |
| | MOTA | 2434 | CA ASN R 26 | | 12.533 -31.017 | 1.00 61.43 | R | C |
| | MOTA | 2435 | CB ASN R 26 | | 11.064 -31.500 | 1.00 60.70 | Ŕ | C |
| | MOTA | 2436 | CG ASN R 26 | | 10.489 -31.183 | 1.00 61.63 1.00 61.76 | R R | C |
| 25 | ATOM | 2437 | OD1 ASN R 26 | | 11.218 -30.646 9.190 -31.394 | 1.00 61.76 | R | N |
| | ATOM | 2438 | ND2 ASN R 26 | | 13.023 -31.342 | 1.00 63.85 | R | C |
| | MOTA MOTA | 2439 2440 | C ASN R 26 O ASN R 26 | | 12.831 -30.585 | 1.00 64.60 | R | ŏ |
| | ATOM | 2441 | O ASN R 26 N ASN R 26 | | 13.722 -32.460 | 1.00 66.73 | R | N |
| 30 | ATOM | 2442 | CA ASN R 26 | | 14.154 -33.058 | 1.00 69.50 | R | Ĉ |
| 30 | ATOM | 2443 | CB ASN R 26 | | 15.589 -33.554 | 1.00 71.22 | R | Č |
| | ATOM | 2444 | CG ASN R 26 | | 16.255 -33.675 | 1.00 73.17 | R | C |
| | MOTA | 2445 | OD1 ASN R 26 | | 15.938 -34.546 | 1.00 74.20 | R | 0 |
| | ATOM | 2446 | ND2 ASN R 26 | | 17.204 -32.755 | 1.00 73.74 | R | N |
| 35 | ATOM | 2447 | C ASN R 26 | | 13.248 -34.221 | 1.00 71.29 | R | С |
| | ATOM | 2448 | O ASN R 26 | 6 12.975 | 13.234 -35.275 | 1.00 70.99 | R | 0 |
| | ATOM | 2449 | N SER R 26 | | 12.431 -33.987 | 1.00 73.90 | R | N |
| | MOTA | 2450 | CA SER R 26 | | 11.511 -35.034 | 1.00 76.24 | R | C |
| | MOTA | 2451 | CB SER R 26 | | 10.618 - 34.462 | 1.00 76.17 | R | C |
| 40 | MOTA | 2452 | OG SER R 26 | | 10.204 -33.149 | 1.00 78.71 | R | 0 |
| | MOTA | 2453 | C SER R 26 | | 12.269 -36.255 | 1.00 77.66 | R | C |
| | ATOM | 2454 | O SER R 26 | | 11.773 -37.370 | 1.00 78.45 1.00 79.01 | R R | N |
| | MOTA | 2455 | N GLN R 26 CA GLN R 26 | | 13.507 -35.990 14.312 -37.060 | 1.00 79.01 | R | C |
| 45 | MOTA MOTA | 2456 2457 | CA GLN R 26 CB GLN R 26 | | 15.459 -36.429 | 1.00 83.07 | | Č |
| 45 | ATOM | 2457 | CG GLN R 26 | | 15.013 -35.922 | 1.00 86.65 | R | č |
| | ATOM | 2459 | CD GLN R 26 | | 16.235 -35.535 | 1.00 88.88 | R | č |
| | MOTA | 2460 | OE1 GLN R 26 | | 16.191 -35.127 | 1.00 89.31 | R | Ō |
| | MOTA | 2461 | NE2 GLN R 26 | | 17.380 -35.696 | 1.00 89.89 | R | N |
| 50 | ATOM | 2462 | C GLN R 26 | | 14.852 -38.017 | 1.00 81.08 | R | С |
| | MOTA | 2463 | O GLN R 26 | | 14.664 -39.228 | 1.00 81.44 | R | 0 |
| | ATOM | 2464 | N THR R 26 | 9 11.368 | 15.591 -37.453 | 1.00 80.39 | R | N |
| | ATOM | 2465 | CA THR R 26 | | 16.091 -38.304 | 1.00 78.88 | R | C |
| | MOTA | 2466 | CB THR R 26 | | 17.415 -37.738 | 1.00 79.42 | R | C |
| 55 | MOTA | 2467 | OG1 THR R 26 | | 17.219 - 36.420 | 1.00 79.08 | R | 0 |
| | MOTA | 2468 | CG2 THR R 26 | | 18.446 -37.673 | 1.00 78.99 | R | C |
| | MOTA | 2469 | C THR R 26 | | 15.049 -38.477 | 1.00 77.19 | R | C |
| | MOTA | 2470 | O THR R 26 | | 14.995 -39.482 | 1.00 76.91 | R | 0 |
| | ATOM | 2471 | N GLUR 2 | | 14.183 -37.451 | 1.00 75.45 | R R | N |
| 60 | ATOM | 2472 | CA GLUR 2 | | | 1.00 73.85 1.00 76.06 | R | C |
| | MOTA | 2473 | CB GLU R 2 | | | 1.00 70.00 | R | C |
| | MOTA | 2474 | CG GLU R 2 | | 11.241 -39.154 10.783 -40.487 | 1.00 79.07 | R | C |
| | MOTA | 2475 | CD GLU R 2' OE1 GLU R 2' | | | 1.00 80.02 | R | Ö |
| 65 | ATOM ATOM | 2476 2477 | OE2 GLU R 2 | | | 1.00 81.18 | R | ŏ |
| 00 | ATOM | 2477 | C GLU R 2' | | | 1.00 71.07 | R | č |
| | ATOM | 2479 | O GLUR 2 | | | 1.00 69.75 | R | Ö |
| | ATOM | 2480 | N THR R 2' | | | 1.00 68.27 | R | \mathbf{N} |
| | ATOM | 2481 | CA THR R 2 | | | 1.00 66.22 | R | С |
| | = " | | | | | | | |

| | ATOM | 2482 | СВ | THR R | 2.11 | ±6.966 | 16.889 -35.574 | 1.00 67.03 | т | R C |
|----|--------------|----------------|-----------|-------|-------|------------------|----------------------------------|--------------------------|---------|-----|
| | ATOM | 2483 | OG1 | | | 17.016 | 17.518 -36.856 | 1.00 69.01 | | R C |
| | ATOM | 2484 | CG2 | THR R | | 18.059 | 17.487 -34.685 | 1.00 66.87 | | R C |
| | MOTA | 2485 | C | THR R | | 17.481 | 14.743 -34.389 | 1.00 63.55 | | . C |
| 5 | MOTA | 2486 | 0 | THR R | 271 | 16.584 | 14.416 -33.623 | 1.00 62.52 | | 3 0 |
| | MOTA | 2487 | N | HIS R | . 272 | 18.743 | 14.504 -34.137 | 1.00 62.01 | | R N |
| | MOTA | 2488 | CA | HIS R | 272 | 19.355 | 13.780 -33.016 | 1.00 60.41 | | R C |
| | ATOM | 2489 | CB | HIS R | 272 | 20.146 | 12.614 -33.522 | 1.00 60.09 | | R C |
| | ATOM | 2490 | CG | HIS R | | 20.925 | 11.930 -32.476 | 1.00 64.26 | | R C |
| 10 | MOTA | 2491 | | HIS R | | 20.641 | 11.652 -31.186 | 1.00 65.40 | F | R C |
| | ATOM | 2492 | | HIS R | | 22.234 | 11.563 - 32.644 | 1.00 66.46 | F | R N |
| | MOTA | 2493 | | HIS R | | 22.721 | 11.079 -31.508 | 1.00 66.77 | F | R C |
| | MOTA | 2494 | | HIS R | | 21.753 | 11.080 -30.622 | 1.00 65.74 | F | R N |
| | ATOM | 2495 | C | HIS R | | 20.212 | 14.860 -32.362 | 1.00 58.50 | F | R C |
| 15 | ATOM | 2496 | 0 | HIS R | | 21.117 | 15.411 - 32.924 | 1.00 57.95 | F | R O |
| | ATOM | 2497 | N | ASN R | | 19.853 | 15.196 -31.198 | 1.00 56.75 | | S N |
| | ATOM | 2498 | CA | ASN R | | 20.636 | 16.051 -30.290 | 1.00 56.29 | F | |
| | MOTA | 2499 | CB | ASN R | | 19.719 | 17.140 -29.794 | 1.00 57.24 | | R C |
| 20 | MOTA MOTA | 2500 2501 | CG OD1 | ASN R | | 19.529 18.437 | 18.290 -30.791 | 1.00 59.20 | | S C |
| 20 | ATOM | 2501 | | ASN R | | 20.618 | 18.683 -31.010 18.821 -31.401 | 1.00 60.99 | F | |
| | ATOM | 2502 | C | ASN R | | 21.205 | 18.821 -31.401 15.359 -28.972 | 1.00 61.33 1.00 54.78 | | N S |
| | ATOM | 2504 | Õ | ASN R | | 20.592 | 14.472 -28.332 | 1.00 54.78 | F | R C |
| | ATOM | 2505 | N | VAL R | | 22.395 | 15.849 -28.533 | 1.00 54.00 | F | - |
| 25 | MOTA | 2506 | CA | VAL R | | 23.079 | 15.410 -27.426 | 1.00 49.18 | F | |
| | ATOM | 2507 | CB | VAL R | | 24.216 | 14.505 -27.781 | 1.00 49.10 | F | |
| | MOTA | 2508 | | VAL R | | 24.845 | 14.060 -26.519 | 1.00 47.67 | F | _ |
| | ATOM | 2509 | | VAL R | | 23.756 | 13.114 -28.509 | 1.00 47.62 | F | |
| | ATOM | 2510 | С | VAL R | 274 | 23.485 | 16.648 -26.596 | 1.00 48.00 | F | |
| 30 | ATOM | 2511 | 0 | VAL R | 274 | 24.321 | 17.401 -27.074 | 1.00 48.15 | F | |
| | MOTA | 2512 | N | PHE R | 275 | 22.898 | 16.838 -25.430 | 1.00 46.02 | F | |
| | MOTA | 2513 | CA | PHE R | | 23.223 | 17.997 -24.604 | 1.00 46.97 | F | S C |
| | MOTA | 2514 | CB | PHE R | | 22.043 | 18.598 -23.942 | 1.00 45.65 | F | ₹ C |
| | MOTA | 2515 | CG | PHE R | | 21.058 | 19.190 -24.895 | 1.00 47.42 | F | |
| 35 | MOTA | 2516 | | PHE R | | 20.129 | 18.361 -25.638 | 1.00 46.46 | F | |
| | ATOM | 2517 | | PHE R | | 21.162 | 20.508 -25.191 | 1.00 46.21 | F | |
| | ATOM | 2518 | | PHE R | | 19.178 | 18.931 -26.577 | 1.00 46.27 | F | |
| | ATOM | 2519 | | PHE R | | 20.316 | 21.057 -26.240 | 1.00 45.90 | F | _ |
| 40 | MOTA | 2520 | CZ | PHE R | | 19.245 | 20.320 -26.842 | 1.00 46.37 | F | |
| 40 | ATOM ATOM | 2521 2522 | C | PHE R | | 24.080 | 17.489 -23.421 | 1.00 48.11 | F | |
| | ATOM | 2523 | N | TYR R | | 23.804 25.205 | 16.462 -22.790 18.120 -23.289 | 1.00 47.90 | F | |
| | ATOM | 2524 | CA | TYR R | | 26.132 | 17.892 -22.206 | 1.00 48.11 1.00 49.41 | A A | - |
| | ATOM | 2525 | CB | TYR R | | 27.556 | 18.113 -22.781 | 1.00 49.41 | F | - |
| 45 | ATOM | 2526 | CG | TYR R | | 28.687 | 17.896 -21.890 | 1.00 52.00 | F | |
| | ATOM | 2527 | CD1 | | | 29.180 | 18.909 -21.024 | 1.00 53.82 | F | |
| | ATOM | 2528 | CE1 | | | 30.356 | 18.592 -20.072 | 1.00 54.29 | F | |
| | ATOM | 2529 | CD2 | TYR R | 276 | 29.218 | 16.669 -21.773 | 1.00 52.53 | F | |
| | ATOM | 2530 | CE2 | | | 30.255 | 16.322 -20.863 | 1.00 53.11 | R | |
| 50 | ATOM | 2531 | CZ | TYR R | 276 | 30.780 | 17.252 -19.988 | 1.00 54.24 | R | |
| | MOTA | 2532 | OH | TYR R | | 31.868 | 16.862 -19.341 | 1.00 56.13 | R | |
| | MOTA | 2533 | С | TYR R | | 25.880 | 18.902 -21.133 | 1.00 49.44 | R | S C |
| | MOTA | 2534 | 0 | TYR R | | 26.056 | 20.049 -21.242 | 1.00 47.42 | R | 0 |
| | ATOM | 2535 | N | VAL R | | 25.490 | 18.395 -19.987 | 1.00 51.00 | R | |
| 55 | ATOM | 2536 | CA | VAL R | | 25.051 | 19.280 -18.964 | 1.00 52.54 | R | |
| | ATOM | 2537 | CB | VAL R | | 23.458 | 19.284 -18.838 | 1.00 53.05 | R | |
| | MOTA | 2538 | | VAL R | | 22.640 | 18.569 -19.923 | 1.00 51.02 | R | |
| | MOTA | 2539 | | VAL R | | 22.965 | 19.091 -17.483 | 1.00 52.55 | R | |
| 60 | MOTA | 2540 | C | VAL R | | 25.751 | 19.142 -17.613 | 1.00 54.64 | R | |
| 60 | ATOM ATOM | $2541 \\ 2542$ | O NT | VAL R | | 25.862 26.333 | 18.026 -17.077 | 1.00 53.39 | R | |
| | | | N | GLN R | | | 20.223 -17.123 | 1.00 57.64 | R | |
| | ATOM ATOM | 2543 2544 | CA CB | GLN R | | 27.081 28.210 | 20.216 -15.792 | 1.00 60.92 | R | |
| | ATOM | 2545 | CG | GLN R | | 28.210 | 21.082 -15.824 21.292 -17.239 | 1.00 62.64 | R cr | |
| 65 | ATOM | 2546 | CD | GLN R | | 30.278 | 21.646 -17.406 | 1.00 66.68 1.00 68.72 | R R | |
| | ATOM | 2547 | OE1 | GLN R | | 31.062 | 21.601 -16.435 | 1.00 69.80 | r R | |
| | MOTA | 2548 | NE2 | GLN R | | 30.682 | 22.000 -18.645 | 1.00 69.14 | R | |
| | ATOM | 2549 | C | GLN R | | 26.264 | 20.455 -14.545 | 1.00 61.75 | R | |
| | ATOM | 2550 | ŏ | GLN R | | 26.522 | 20.013 -13.532 | 1.00 61.88 | R | |
| | | | | | | | | | | _ |

| | " ATOM | 2551 | N | GLU R 279 | 25.160 | 21.102 -14.739 | 1.00 63.48 | R | N |
|-----|--------------|--------------|----------|--------------------------|------------------|----------------------------------|--------------------------|--------|--------|
| | ATOM | 2552 | CA | GLU R 279 | 24.333 | 21.641 -13.721 | 1.00 65.20 | R | C |
| | MOTA | 2553 | CB | GLU R 279 | 24.469 | 23.152 -13.731 | 1.00 65.02 1.00 66.40 | R R | C |
| - | ATOM | 2554 2555 | C | GLU R 279 GLU R 279 | 22.905 22.318 | 21.254 -14.034 21.601 -15.055 | 1.00 66.33 | R | Ö |
| 5 | ATOM ATOM | 2556 | И | ALA R 280 | 22.345 | 20.440 -13.145 | 1.00 68.12 | R | N |
| | ATOM | 2557 | CA | ALA R 280 | 20.986 | 20.030 -13.386 | 1.00 70.55 | R | C |
| | MOTA | 2558 | CB | ALA R 280 | 20.995 | 18.527 -13.699 | 1.00 68.51 | R R | C |
| | ATOM | 2559 | C | ALA R 280 | 20.177 19.634 | 20.253 -12.142 19.327 -11.575 | 1.00 72.94 1.00 72.68 | R | Ö |
| 10 | MOTA MOTA | 2560 2561 | И О | ALA R 280 LYS R 281 | 20.159 | 21.537 -11.689 | 1.00 75.96 | R | N |
| | ATOM | 2562 | CA | LYS R 281 | 19.418 | 21.812 -10.474 | 1.00 79.54 | R | C |
| | ATOM | 2563 | СВ | LYS R 281 | 19.816 | 23.160 -9.886 | 1.00 79.86 | R | C |
| | MOTA | 2564 | CG | LYS R 281 | 19.897 | 23.025 -8.363 | 1.00 80.01 | R | C |
| 15 | MOTA | 2565 | CD | LYS R 281 | 20.945 22.361 | 23.937 -7.726 23.389 -7.882 | 1.00 79.40 1.00 79.46 | R R | C |
| | MOTA | 2566 2567 | CE NZ | LYS R 281 LYS R 281 | 23.266 | 24.502 -8.130 | 1.00 79.43 | R | N |
| | MOTA MOTA | 2568 | C | LYS R 281 | 17.923 | 21.719 -10.689 | 1.00 82.08 | R | C |
| | MOTA | 2569 | ŏ | LYS R 281 | 17.290 | 22.454 -11.445 | 1.00 81.67 | R | 0 |
| 20 | MOTA | 2570 | N | CYS R 282 | 17.338 | 20.710 -10.049 | 1.00 84.54 | R | N |
| | MOTA | 2571 | CA | CYS R 282 | 15.930 | 20.563 -10.411 21.633 -9.740 | 1.00 86.72 1.00 88.49 | R R | C |
| | MOTA | 2572 2573 | C O | CYS R 282 CYS R 282 | 15.074 14.287 | 21.367 -8.834 | 1.00 89.72 | R | ŏ |
| | MOTA MOTA | 2574 | CB | CYS R 282 | 15.473 | 19.183 -9.941 | 1.00 86.35 | R | C |
| 25 | MOTA | 2575 | SG | CYS R 282 | 14.708 | 18.208 -11.254 | 1.00 88.45 | R | S |
| | MOTA | 2576 | N | GLU R 283 | 15.265 | 22.886 -10.178 | 1.00 90.11 | R | И |
| | MOTA | 2577 | CA | GLU R 283 | 14.567 14.600 | 23.943 -9.463 23.581 -7.981 | 1.00 92.03 1.00 92.46 | R R | C |
| | MOTA | 2578 2579 | CB CG | GLU R 283 GLU R 283 | 14.683 | 24.814 -7.078 | 1.00 93.73 | R | Č |
| 30 | ATOM ATOM | 2580 | CD | GLU R 283 | 13.454 | 25.660 -7.294 | 1.00 95.07 | R | C |
| 00 | ATOM | 2581 | OE1 | GLU R 283 | 13.554 | 26.872 - 7.195 | 1.00 95.36 | R | 0 |
| | MOTA | 2582 | | GLU R 283 | 12.407 | 25.093 -7.596 | 1.00 95.10 | R R | 0 |
| | ATOM | 2583 | C | GLU R 283 | 15.219 16.389 | 25.319 -9.637 25.531 -9.343 | 1.00 93.03 1.00 93.42 | R R | 0 |
| 25 | MOTA | 2584 2585 | N O | GLU R 283 ASN R 284 | 14.440 | 26.266 -10.203 | 1.00 94.22 | R | Ŋ |
| 35 | ATOM ATOM | 2586 | CA | ASN R 284 | 13.147 | 25.899 -10.787 | 1.00 95.83 | R | С |
| | ATOM | 2587 | CB | ASN R 284 | 12.279 | 27.158 -10.865 | 1.00 95.79 | R | C |
| | ATOM | 2588 | C | ASN R 284 | 13.304 | 25.291 -12.185 | 1.00 97.36 | R R | C O |
| 4.0 | ATOM | 2589 | 0 | ASN R 284 | 14.158 12.396 | 24.452 -12.440 25.707 -13.095 | 1.00 98.00 1.00 98.24 | R | И |
| 40 | MOTA MOTA | 2590 2591 | N CD | PRO R 285 PRO R 285 | 12.412 | 25.484 -14.529 | 1.00 98.86 | R | Ĉ |
| | ATOM | 2592 | CA | PRO R 285 | 11.267 | 26.543 -12.732 | 1.00 99.16 | R | C |
| | ATOM | 2593 | CB | PRO R 285 | 10.547 | | 1.00 98.54 | R | C |
| | MOTA | 2594 | CG | PRO R 285 | 11.139 | | 1.00 98.67 1.00 99.89 | R R | C |
| 45 | ATOM | 2595 | C | PRO R 285 PRO R 285 | 10.275 10.314 | | 1.00 99.89 | R | Õ |
| | ATOM ATOM | 2596 2597 | N O | | 9.353 | | 1.00100.79 | R | Ŋ |
| | MOTA | 2598 | CA | GLU R 286 | 8.546 | | 1.00102.10 | R | C |
| | ATOM | 2599 | CB | GLU R 286 | 8.208 | | 1.00103.19 | R | C |
| 50 | MOTA | 2600 | CG | GLU R 286 | 9.398 | | 1.00106.31 1.00109.22 | R R | C |
| | MOTA | 2601 | CD | GLU R 286 1 GLU R 286 | 9.043 8.023 | | 1.00109.22 | R | Õ |
| | MOTA MOTA | 2602 2603 | OE: | | 9.891 | | 1.00109.63 | R | 0 |
| | ATOM | 2604 | C. | GLU R 286 | 7.297 | | 1.00101.95 | R | C |
| 55 | MOTA | 2605 | 0 | GLU R 286 | 6.579 | | 1.00102.44 | R | O |
| | MOTA | 2606 | N | PHE R 287 | 7.049 | | 1.00101.53 1.00101.39 | R R | N C |
| | MOTA | 2607 2608 | CA | PHE R 287 PHE R 287 | 6.017 6.246 | | 1.00101.33 | R | č |
| | MOTA MOTA | 2609 | CB CG | | 5.519 | | 1.00100.24 | R | C |
| 60 | ATOM | 2610 | | 1 PHE R 287 | 5.083 | 26.324 -13.787 | 1.00100.27 | R | C |
| | MOTA | 2611 | CD | 2 PHE R 287 | 5.407 | | 1.00 99.82 | R | C |
| | ATOM | 2612 | | 1 PHE R 287 | 4.554 | | 1.00100.42 1.00 99.79 | R R | C |
| | MOTA | 2613 | CE | | 4.877 4.453 | | 1.00 99.79 | R R | C |
| 65 | MOTA MOTA | 2614 2615 | CZ C | PHE R 287 | 6.231 | | 1.00101.27 | R | С |
| 00 | ATOM | 2616 | Õ | PHE R 287 | 5.662 | 22.768 -10.455 | 1.00101.94 | R | 0 |
| | MOTA | 2617 | N | GLU R 288 | 7.071 | | 1.00100.02 | R | N |
| | MOTA | 2618 | CA | | 7.559 | | 1.00 98.61 1.00 98.36 | R R | C |
| | ATOM | 2619 | СВ | GLU R 288 | 8.364 | . 20.000 -I3.IO3 | 1.00 20.30 | 14 | Ŭ |

| | ATOM | 2620 | CG | GLU R | 200 | 0 | .288 | 21 662 | -14.287 | 1 00 | 96.79 | ъ | ~ |
|-----|------|------|------------------|-------|--------|-----|-------|--------|---------|------------|-------|----|---|
| | | | | | | | | | | | | R | C |
| | ATOM | 2621 | CD | GLU R | | | .189 | 21.296 | -15.253 | | 96.23 | R | C |
| | ATOM | 2622 | OE1 | GLU R | 288 | 6 | .418 | 20.383 | -14.968 | 1.00 | 95.74 | R | 0 |
| | ATOM | 2623 | OE2 | GLU R | 288 | 7 | .114 | 21.939 | -16.289 | 100 | 95.82 | R | 0 |
| 5 | ATOM | 2624 | С | GLU R | | | .475 | | -10.695 | | 98.28 | R | č |
| Ū | ATOM | 2625 | | GLU R | | | | | | | | | |
| | | | 0 | - | | | .806 | 21.999 | -10.105 | | 99.09 | R | 0 |
| | ATOM | 2626 | \mathbf{N} | ASN R | 293 | 1.5 | .776 | 13.988 | -4.556 | 1.00 | 96.30 | R | N |
| | ATOM | 2627 | CA | ASN R | 293 | 1.6 | .678 | 13.056 | -5.247 | 1 00 | 94.19 | R | C |
| | ATOM | 2628 | СВ | ASN R | | | .082 | 11.655 | | | | | |
| 4.0 | | | | | | | | | -5.105 | | 94.17 | R | C |
| 10 | ATOM | 2629 | C | ASN R | | | .848 | 13.400 | -6.723 | 1.00 | 93.16 | R | C |
| | ATOM | 2630 | 0 | ASN R | 293 | 17 | .584 | 12.788 | -7.497 | 1.00 | 93.06 | R | 0 |
| | ATOM | 2631 | N | THR R | | 16 | .059 | 14.403 | -7.132 | | 91.21 | R | N |
| | ATOM | 2632 | CA | | | | | | | | | | |
| | | | | THR R | | | .794 | 14.564 | -8.540 | | 89.29 | R | C |
| | ATOM | 2633 | CB | THR R | 294 | 14 | .284 | 14.787 | -8.711 | 1.00 | 89.60 | R | C |
| 15 | ATOM | 2634 | OG1 | THR R | 294 | 13 | .617 | 13.719 | -8.060 | 1.00 | 90.25 | R | 0 |
| | ATOM | 2635 | CG2 | | | 13 | .874 | 14.837 | | | 89.47 | R | |
| | | | | | | | | | | | | | C |
| | ATOM | 2636 | C | THR R | | | .596 | 15.682 | -9.162 | | 87.98 | R | С |
| | MOTA | 2637 | 0 | THR R | 294 | 17 | .329 | 16.461 | -8.558 | 1.00 | 88.24 | R | 0 |
| | ATOM | 2638 | N | SER R | 295 | 1.6 | .502 | 15.680 | -10.483 | 1 00 | 85.90 | R | N |
| 20 | ATOM | 2639 | CA | SER R | | | .297 | | -11.209 | | | | |
| 20 | | | | | | | | | | | 83.53 | R | C |
| | ATOM | 2640 | CB | SER R | | T8 | .671 | | -11.391 | 1.00 | 83.77 | R | C |
| | ATOM | 2641 | OG | SER R | 295 | 19 | .141 | 15.529 | -10.111 | 1.00 | 83.53 | R | 0 |
| | MOTA | 2642 | C | SER R | 2.95 | 16 | .643 | 16.780 | -12.538 | 1 00 | 81.72 | R | C |
| | ATOM | 2643 | ŏ | SER R | | | .926 | | | | | | |
| 0.5 | | | | | | | | | -12.998 | | 81.17 | R | 0 |
| 25 | MOTA | 2644 | N | CYS R | | | .885 | 17.964 | -13.112 | 1.00 | 80.55 | R | N |
| | ATOM | 2645 | $^{\rm CA}$ | CYS R | 296 | 16 | .281 | 18.168 | -14.431 | 1.00 | 79.65 | R | C |
| | ATOM | 2646 | С | CYS R | 296 | 16 | .939 | | -15.191 | | 77.11 | R | Č |
| | | | | | | | | | | | | | |
| | ATOM | 2647 | 0 | CYS R | | | .746 | | -14.657 | | 76.87 | R | 0 |
| | ATOM | 2648 | $^{\mathtt{CB}}$ | CYS R | 296 | 14 | .793 | 18.467 | -14.245 | 1.00 | 82.55 | R | C |
| 30 | ATOM | 2649 | SG | CYS R | 296 | 14 | .487 | 19,494 | -12.793 | 1.00 | 87.30 | R | S |
| | ATOM | 2650 | N | PHE R | | | .583 | | -16.478 | | 74.68 | R | Ñ |
| | | | | | | | | | | | | | |
| | MOTA | 2651 | ca | PHE R | | | .301 | | -17.437 | | 72.94 | R | C |
| | ATOM | 2652 | CB | PHE R | 297 | 18 | .463 | 19.266 | -17.930 | 1.00 | 69.47 | R | C |
| | ATOM | 2653 | CG | PHE R | 297 | 18 | .954 | 19.781 | -19.242 | 1.00 | 66.15 | R | C |
| 35 | ATOM | 2654 | | PHE R | | | .634 | | -19.284 | | - | | ~ |
| 33 | | | | | | | | | | | 64.52 | R | C |
| | ATOM | 2655 | CD2 | | | | .663 | | -20.408 | 1.00 | 65.09 | R | С |
| | ATOM | 2656 | CE1 | PHE R | 297 | 20 | .028 | 21.514 | -20.507 | 1.00 | 63.49 | R | C |
| | ATOM | 2657 | CE2 | PHE R | 297 | 19 | .061 | 19 625 | -21.633 | 1 00 | 64.98 | R | C |
| | ATOM | 2658 | CZ | PHE R | | | | | | | | | |
| 40 | | | | | | | .742 | | -21.686 | | 63.88 | R | C |
| 40 | MOTA | 2659 | C | PHE R | | 16 | .370 | 20.482 | -18.598 | 1.00 | 73.41 | R | C |
| | ATOM | 2660 | 0 | PHE R | 297 | 15 | .776 | 19.621 | -19.241 | 1.00 | 73.80 | R | 0 |
| | ATOM | 2661 | N | MET R | 298 | 16 | .197 | | -18.807 | | 74.36 | R | N |
| | | | | | | | | | | | | | |
| | MOTA | 2662 | CA | MET R | | | .244 | | -19.825 | | 74.98 | R | C |
| | MOTA | 2663 | CB | MET R | 298 | 14 | .809 | | -19.491 | 1.00 | 78.07 | R | C |
| 45 | MOTA | 2664 | CG | MET R | 298 | 13 | .351 | 23.736 | -19.032 | 1.00 | 81.75 | R | C |
| | ATOM | 2665 | SD | MET R | 298 | 12 | .238 | | -20.368 | | 87.08 | R | s |
| | | | | | | | | | -19.817 | | | | |
| | ATOM | 2666 | CE | MET R | | | .798 | | | | 85.81 | R | С |
| | ATOM | 2667 | C | MET R | | 15 | .850 | 22.186 | -21.235 | 1.00 | 73.57 | R | С |
| | MOTA | 2668 | 0 | MET R | 298 | 16 | .835 | 22.840 | -21.542 | 1.00 | 72.23 | R | 0 |
| 50 | ATOM | 2669 | N | VAL R | | | .243 | | -22.087 | | 73.62 | R | N |
| | ATOM | 2670 | CA | VAL R | | | .682 | | | | | | |
| | | | | | | | | | -23.476 | | 74.43 | R | C |
| | MOTA | 2671 | CB | VAL R | 299 | 15 | .274 | 19.896 | -24.016 | 1.00 | 74.27 | R | C |
| | ATOM | 2672 | CG1 | VAL R | 299 | 15 | .621 | 19.794 | -25.502 | 1.00 | 73.21 | R | C |
| | ATOM | 2673 | | VAL R | | | .969 | | -23.253 | | 73.35 | | Č |
| EE | | | | | | | | | | | | R | C |
| 55 | ATOM | 2674 | C | VAL R | | | .984 | | -24.307 | | 75.41 | R | C |
| | ATOM | 2675 | 0 | VAL R | 299 | 13 | .754 | 22.362 | -24.417 | 1.00 | 76.00 | R | 0 |
| | ATOM | 2676 | N | PRO R | 300 | 15 | .766 | 23 256 | -24.877 | 1 00 | 76.10 | R | N |
| | ATOM | 2677 | CD | PRO R | | | .231 | 23 367 | -24.920 | | | | |
| | | | | | | | | | | | 75.65 | R | C |
| | ATOM | 2678 | ca | PRO R | | | .182 | | -25.621 | 1.00 | 76.85 | R | C |
| 60 | ATOM | 2679 | CB | PRO R | 300 | 16 | .211 | 25.445 | -25.714 | 1.00 | 75.84 | R | C |
| | ATOM | 2680 | CG | PRO R | 300 | | .584 | | -25.326 | | 76.48 | R | Č |
| | ATOM | 2681 | Č | PRO R | | | .788 | | | | | | |
| | | | | | | | | | -27.029 | | 77.72 | R | C |
| | ATOM | 2682 | 0 | PRO R | | | .439 | | -27.659 | | 77.18 | R | 0 |
| | ATOM | 2683 | N | GLY R | 301 | 13 | .653 | 24.369 | -27.508 | 1.00 | 79.03 | R | N |
| 65 | ATOM | 2684 | CA | GLY R | | | .330 | | -28.925 | | 80.40 | R | Ċ |
| | ATOM | 2685 | | GLY R | | | | | | | | | |
| | | | C | | | | .452 | | -29.217 | | 82.28 | R | C |
| | ATOM | 2686 | 0 | GLY R | | | .762 | | -30.061 | | 82.07 | R | 0 |
| | ATOM | 2687 | \mathbf{N} | VAL R | 302 | 11. | .340 | 22.803 | -28.482 | 1.00 | 83.95 | R | N |
| | ATOM | 2688 | CA | VAL R | | | .336 | | -28.727 | | 86.24 | R | Ĉ |
| | | | | , 10 | 2 3 23 | | - 550 | | 20.121 | 00 | 00.44 | 1. | · |

| | ATOM 2689 CB VAL R 302 | 10.530 20.719 -27.697 1.00 85.51 10.253 19.323 -28.323 1.00 84.83 | R C R C |
|----|---|--|------------|
| | ATOM 2690 CG1 VAL R 302 | 10.253 19.323 -20.325 1.00 84.47 | R C R C |
| | ATOM 2692 C VAL R 302 | 8.905 22.505 29.002 1.00 88.68 | R O |
| 5 | ATOM 2693 O VAL R 302 ATOM 2694 N LEU R 303 | 7.882 21.462 -28.616 1.00 90.03 | R N R C |
| | ATOM 2695 CA LEU R 303 | 6.591 21.538 23.422 1.00 92.45 | R C |
| | ATOM 2696 CB LEU R 303 | 7.913 20.421 -31.277 1.00 93.46 | R C R C |
| 10 | AUDIN 2698 CD1 LEU R 303 | 7.925 15.110 22 104 1 00 93 79 | R C |
| 10 | ATOM 2699 CD2 LEU R 303 | 5.161 21.816 -28.787 1.00 92.36 | R C R O |
| | ATOM 2701 O LEU R 303 | 5.009 22.832 -28.151 1.00 92.58 4.117 20.908 -28.913 1.00 92.77 | R N |
| | ATOM 2702 N PRO R 304 | 2.701 21.191 -29.072 1.00 93.52 | R C R C |
| 15 | ATOM 2704 CA PRO R 304 | 4.243 19.458 -28.646 1.00 92.92 | R C R C |
| | ATOM 2705 CB PRO R 304 | 1.005 20.024 -28.339 1.00 93.42 | R C |
| | ATOM 2706 CG PRO R 304 ATOM 2707 C PRO R 304 | 4.280 18.542 -29.935 1.00 92.84 | R C R O |
| 20 | ATIOM 2708 O PRO R 304 | 5.300 17.532 -30.664 1.00 92.50 | R N |
| | ATOM 2709 N ASP R 305 | 5 465 18.034 -32.072 1.00 91.71 | R C R C |
| | ATOM 2711 CB ASP R 305 | 6.433 16.389 -32.066 1.00 90.87 | R C |
| | ATOM 2712 C ASP R 305 | 7 420 16.623 -32.600 1.00 91.22 | R O R N |
| 25 | ATTOM 2714 N THR R 306 | 6.020 16.044 -30.999 1.00 89.25 6.861 15.107 -30.538 1.00 87.16 | R C |
| | ATOM 2715 CA THR R 306 | 6 120 15.104 -29.244 1.00 87.79 | R C R C |
| | ATOM 2717 C THR R 306 | 6.536 14.110 -31.632 1.00 85.00 | R O |
| 30 | ATOM 2718 O THR R 306 | 6.647 12.740 -31.554 1.00 83.46 | R N R C |
| | ATOM 2720 CA LEU R 307 | 7.670 12.045 -30.710 1.00 81.38 | R C R C |
| | ATOM 2721 CB LEU R 307 | 7 911 9.727 -30.735 1.00 84.50 | R C |
| | ATOM 2722 CG LEU R 307 ATOM 2723 CD1 LEU R 307 | 7.057 9.946 -29.505 1.00 85.37 | R C R C |
| 35 | ATOM 2724 CD2 LEU R 307 | 7.478 8.434 31.112 1.00 78.72 | R C |
| | ATOM 2725 C LEU R 307 ATOM 2726 O LEU R 307 | 9 802 12.910 -31.602 1.00 77.76 | R O R N |
| | ATOM 2727 N ASN R 308 | 9.241 13.110 -29.379 1.00 74.87 10.604 13.198 -28.882 1.00 70.88 | R C |
| 40 | ATOM 2728 CA ASN R 308 | 10.764 14.553 -28.180 1.00 71.05 | R C R C |
| | ATOM 2730 CG ASN R 308 | 10.584 15.600 25.100 1 00 69 42 | R O |
| | ATOM 2731 OD1 ASN R 308 | 9.330 16.145 -29.307 1.00 72.76 | R N R C |
| 45 | AUDOM 2733 C ASN R 308 | 10.837 12.039 -27.921 1.00 67.32 | R O |
| 70 | ATOM 2734 O ASN R 308 | 11 943 11.335 -28.154 1.00 63.68 | R N R C |
| | ATOM 2736 CA THR R 309 | 12.474 10.361 -27.219 1.00 60.57 | R C |
| | ATOM 2737 CB THR R 309 | 11 548 8.609 -28.443 1.00 61.79 | R O R C |
| 50 | ATOM 2739 CG2 THR R 309 | 13.202 8.074 -26.978 1.00 60.41 | R C |
| | ATOM 2740 C THR R 309 | 14.518 11.399 -27.106 1.00 56.57 | R O R N |
| | ATOM 2742 N VAL R 310 | 13.719 10.662 -25.207 1.00 54.47 | R C |
| 55 | ATOM 2743 CA VAL R 310 | 14.650 12.236 -23.544 1.00 51.82 | R C R C |
| | ATOM 2745 CG1 VAL R 310 | 13.410 12.691 -23.283 1.00 52.41 | r C |
| | ATOM 2746 CG2 VAL R 310 | 15 498 9.854 -23.760 1.00 52.00 | R C R O |
| 00 | ATOM 2747 C VAL R 310 ATOM 2748 O VAL R 310 | 14.832 8.965 -23.452 1.00 51.06 | R O R N |
| 60 | ATOM 2749 N ARG R 311 | 17 636 9 044 -22.827 1.00 50.34 | R C |
| | ATOM 2750 CA ARG R 311 | 18.382 8.071 -23.685 1.00 49.77 | R C R C |
| | ATOM 2752 CG ARG R 311 | 10 225 5 951 -24.887 1.00 48.25 | R C |
| 65 | ATOM 2753 CD ARG R 311 | 19.164 6.449 -25.845 1.00 48.40 | R N R C |
| | ATTOM 2755 CZ ARG R 311 | 20.094 5.686 -26.333 1.00 47.77 | R N |
| | ATOM 2756 NH1 ARG R 311 | 20.286 4.483 -25.817 1.00 47.01 20.930 6.183 -27.166 1.00 44.86 | R N |
| | ATOM 2757 NH2 ARG R 311 | 218 | |

| | | | | | | | _ | ~ |
|------|--------------|----------------|--------------------------------|------------------|----------------------------------|--------------------------|--------|-----------|
| | ATOM | | C ARG R 311 | 18.638 | 9.873 -22.106 | 1.00 50.05 1.00 50.01 | R R | C O |
| | MOTA | | O ARG R 311 | | 10.849 -22.564 9.397 -20.972 | 1.00 30.01 | R | N |
| | MOTA | | N ILE R 312 | 19.005 20.054 | 10.009 -20.194 | 1.00 48.58 | R | Ĉ |
| - | MOTA MOTA | | CA ILE R 312 CB ILE R 312 | 19.425 | 10.760 -18.938 | 1.00 48.15 | R | С |
| 5 | ATOM | | CG2 ILE R 312 | 20.437 | 11.526 -18.285 | 1.00 45.62 | R | C |
| | MOTA | | CG1 ILE R 312 | 18.335 | 11.630 -19.384 | 1.00 47.07 | R | C |
| | MOTA | | CD1 ILE R 312 | 17.552 | 12.196 -18.148 | 1.00 47.91 1.00 47.90 | R R | C C |
| | MOTA | | C ILE R 312 | 21.130 | 9.104 -19.668 8.075 -19.145 | 1.00 47.30 | R | Õ |
| 10 | ATOM | | O ILE R 312 N ARG R 313 | 20.812 22.397 | 9.485 -19.792 | 1.00 46.57 | R | N |
| | MOTA | | N ARG R 313 CA ARG R 313 | 23.455 | 8.761 -19.035 | 1.00 46.06 | R | С |
| | MOTA MOTA | | CB ARG R 313 | 24.443 | 8.114 -20.054 | 1.00 45.95 | R. | C |
| | ATOM | | CG ARG R 313 | 25.120 | 8.994 -20.854 | 1.00 43.85 | R | C |
| 15 | ATOM | | CD ARG R 313 | 25.770 | 8.153 -22.104 | 1.00 45.64 | R | C N |
| | MOTA | | NE ARG R 313 | 26.641 | 8.967 -22.942 8.467 -23.644 | 1.00 47.51 1.00 48.52 | R R | C |
| | MOTA | | CZ ARG R 313 | 27.615 27.780 | 7.223 -23.634 | 1.00 48.93 | R | N |
| | ATOM | | NH1 ARG R 313 NH2 ARG R 313 | 28.440 | 9.211 -24.327 | 1.00 48.72 | R | N |
| 00 | MOTA MOTA | 2776 2777 | NH2 ARG R 313 C ARG R 313 | 24.216 | 9.675 ~18.156 | 1.00 46.35 | R | С |
| 20 | ATOM | 2778 | O ARG R 313 | 24.101 | 10.926 -18.315 | 1.00 44.37 | R - | 0 |
| | MOTA | 2779 | N VAL R 314 | 25.221 | 9.158 -17.462 | 1.00 45.29 | R | N |
| | MOTA | 2780 | CA VAL R 314 | 25.783 | 9.929 -16.364 | 1.00 45.74 1.00 46.13 | R R | C |
| | MOTA | 2781 | CB VAL R 314 | 24.867 | 9.539 -15.130 9.400 -13.942 | 1.00 47.48 | R | č |
| 25 | MOTA | 2782 | CG1 VAL R 314 CG2 VAL R 314 | 25.561 23.644 | 10.474 -15.035 | 1.00 44.87 | R | Ċ |
| | MOTA | 2783 2784 | C VAL R 314 | 27.213 | 9.495 -16.103 | 1.00 45.86 | R | С |
| | ATOM ATOM | 2785 | O VAL R 314 | 27.549 | 8.410 -16.273 | 1.00 45.19 | R | 0 |
| | ATOM | 2786 | N LYS R 315 | 28.012 | 10.410 -15.597 | 1.00 45.17 | R | N |
| 30 | ATOM | 2787 | CA LYS R 315 | 29.411 | 10.186 -15.205 | 1.00 45.60 1.00 45.36 | R R | C C |
| | MOTA | 2788 | CB LYS R 315 | 30.396 | 10.453 -16.373 11.871 -16.660 | 1.00 47.28 | R | č |
| | MOTA | 2789 | CG LYS R 315 CD LYS R 315 | 30.500 31.601 | 12.117 -17.811 | 1.00 47.54 | R | Ċ |
| | ATOM | 2790 2791 | CD LYS R 315 CE LYS R 315 | 31.724 | 13.600 -18.055 | 1.00 48.20 | R | C |
| 35 | MOTA MOTA | 2792 | NZ LYS R 315 | 32.778 | 13.957 -19.216 | 1.00 47.70 | R | \vec{n} |
| 55 | MOTA | 2793 | C LYS R 315 | 29.860 | 10.915 -14.049 | 1.00 44.27 | R | C |
| | ATOM | 2794 | O LYS R 315 | 29.239 | 11.844 -13.662 | 1.00 45.27 1.00 43.47 | R R | N O |
| | MOTA | 2795 | N THR R 316 | 30.993 | 10.563 -13.451 11.337 -12.235 | 1.00 43.47 | R | Ĉ |
| | ATOM | 2796 | CA THR R 316 | 31.399 32.394 | 10.587 -11.331 | 1.00 42.26 | R | Č |
| 40 | MOTA | 2797 2798 | CB THR R 316 OG1 THR R 316 | 33.362 | 10.177 -12.194 | 1.00 42.09 | R | 0 |
| | ATOM ATOM | 2799 | CG2 THR R 316 | 31.767 | 9.355 -10.816 | 1.00 40.88 | R | C |
| | ATOM | 2800 | C THR R 316 | 32.110 | 12.606 -12.705 | 1.00 43.10 | R | C |
| | MOTA | 2801 | O THR R 316 | 32.803 | 12.506 -13.640 | 1.00 41.11 1.00 43.52 | R R | N O |
| 45 | ATOM | 2802 | N ASN R 317 | 31.873 32.661 | 13.816 -12.092 14.997 -12.130 | 1.00 45.32 | R | Ĉ |
| | MOTA | 2803 | CA ASN R 317 CB ASN R 317 | 32.123 | 16.013 -10.778 | 1.00 46.56 | R | C |
| | MOTA ATOM | $2804 \\ 2805$ | CB ASN R 317 CG ASN R 317 | 31.132 | 16.678 -11.276 | 1.00 50.66 | R | C |
| | MOTA | 2806 | OD1 ASN R 317 | 31.227 | 16.780 -12.543 | 1.00 54.75 | R | 0 |
| 50 | ATOM | 2807 | ND2 ASN R 317 | 30.170 | 17.164 -10.603 | 1.00 51.29 1.00 47.72 | R R | C N |
| | ATOM | 2808 | C ASN R 317 | 34.136 | 14.786 -11.786 13.899 -11.074 | | R | ŏ |
| | MOTA | 2809 | O ASN R 317 N LYS R 318 | 34.335 34.945 | 15.799 -11.916 | 1.00 48.90 | R | N |
| | MOTA | 2810 2811 | N LYS R 318 CA LYS R 318 | 36.301 | 15.935 -11.309 | 1.00 50.22 | R | С |
| 55 | ATOM ATOM | 2812 | CB LYS R 318 | 37.303 | 16.666 -12.338 | 1.00 52.02 | R | C |
| 50 | ATOM | 2813 | CG LYS R 318 | 37.001 | 18.223 -12.395 | | R | C |
| | ATOM | 2814 | CD LYS R 318 | 38.028 | 19.020 -13.178 | 1.00 56.69 1.00 60.37 | R R | C |
| | ATOM | 2815 | CE LYS R 318 | 37.332 | 19.973 -14.178 21.279 -14.250 | | R | N |
| (0.5 | ATOM | 2816 | NZ LYS R 318 | 38.027 36.319 | 16.583 -9.871 | | R | C |
| 60 | ATOM | 2817 | C LYS R 318 O LYS R 318 | 37.357 | 16.477 -9.205 | | R | 0 |
| | MOTA MOTA | 2818 2819 | O LYS R 318 N LEU R 319 | 35.118 | 16.836 -9.312 | 1.00 49.14 | R | N |
| | ATOM | 2820 | CA LEU R 319 | 34.979 | 17.469 -8.010 | | R | C |
| | MOTA | 2821 | CB LEU R 319 | 33.815 | 18.468 -8.032 | | R | C |
| 65 | MOTA | 2822 | CG LEU R 319 | 33.842 | 19.321 -9.298 | | R R | C |
| | ATOM | 2823 | CD1 LEU R 319 | 32.549 | 20.109 -9.435 20.362 -9.298 | | R | Ç |
| | MOTA | 2824 | CD2 LEU R 319 C LEU R 319 | 34.945 34.826 | | | R | C |
| | MOTA | | C LEU R 319 O LEU R 319 | 35.153 | 16.826 -5.671 | | R | 0 |
| | ATOM | 2020 | 0 1110 11 313 | 210 | | | | |

| | | | | | | | 45 000 | | 4 00 70 | | _ | |
|----|--------------|--------------|--------|----------------|-----|------------------|-----------------|--------------------|----------------------|----|--------|-----------------|
| | ATOM | 2827 | N | CYS R | - | 34.255 | 15.280 | -7.087 | 1.00 52. | | R | N |
| | MOTA | 2828 | CA | | 320 | 34.143 | 14.287 | -6.015 | 1.00 54. | | R | C |
| | MOTA | 2829 | C | CYS R | | 35.100 | 13.111 | -6.283 | 1.00 54. | - | R | C |
| | MOTA | 2830 | 0_ | CYS R | | 35.793 | 12.594 | -5.408 | 1.00 54. | | R | 0 |
| 5 | MOTA | 2831 | CB | CYS R | | 32.670 | 13.787 | -5.987 | 1.00 54. | | R | C |
| | MOTA | 2832 | SG | CYS R | | 31.444 | 15.094 | -5.670 | 1.00 55. | | R | S |
| | MOTA | 2833 | N | TYR R | | 35.052 | 12.647 | -7.540 | 1.00 55. | | R | \widetilde{N} |
| | MOTA | 2834 | CA | TYR R | | 35.921 | 11.566 | -7.924 | 1.00 57. | | R | C |
| | MOTA | 2835 | CB | TYR R | | 35.038 | 10.437 | -8.520 | 1.00 57. | | R | C |
| 10 | MOTA | 2836 | CG | TYR R | | 34.109 | 9.835 | -7.496 | 1.00 57. | | R | C |
| | MOTA | 2837 | CD1 | | | 34.556 | 8.880 | -6.570 | 1.00 58. | | R | C |
| | MOTA | 2838 | CE1 | | | 33.703 | 8.424 | -5.563 | 1.00 58. | | R | C |
| | MOTA | 2839 | CD2 | | | 32.779 | 10.271 | -7.435 | 1.00 57. | | R | C |
| | MOTA | 2840 | CE2 | | | 31.940 | 9.831 | -6.417 | 1.00 58. | | R | C |
| 15 | ATOM | 2841 | CZ | TYR R | | 32.377 | 8.910 | -5.496 | 1.00 58. | | R | C |
| | ATOM | 2842 | OH | TYR R | | 31.560 | 8.536 | -4.446 | 1.00 60. | | R | 0 |
| | MOTA | 2843 | C | TYR R | | 36.869 | 12.128 | -8.981 | 1.00 58. 1.00 59. | | R | C |
| | MOTA | 2844 | 0 | TYR R | | 37.605 | 13.095 | -8.757 -10.162 | 1.00 60. | | R R | 0 |
| 00 | MOTA | 2845 | N | GLU R | | 36.780 37.583 | 11.530 12.049 | -10.162 | 1.00 60. | | R | N C |
| 20 | ATOM | 2846 | CA | GLU R | | 38.796 | 11.128 | -11.231 -11.294 | 1.00 62. | | R | G |
| | MOTA | 2847 | CB | GLU R GLU R | | 39.983 | | -11.294 -12.070 | 1.00 70. | | R | c |
| | ATOM | 2848 2849 | CD | GLU R | | 41.272 | | -11.396 | 1.00 74. | | R | G |
| | MOTA | 2850 | OE1 | | | 42.167 | | -12.082 | 1.00 77. | | R | Ö |
| 25 | MOTA ATOM | 2851 | OE2 | | | 41.371 | | -10.186 | 1.00 76. | | R | ŏ |
| 23 | ATOM | 2852 | C | GLU R | | 36.754 | | -12.512 | 1.00 61. | | R | č |
| | ATOM | 2853 | Ö | GLU R | | 35.916 | | -12.684 | 1.00 61. | | R | ŏ |
| | ATOM | 2854 | N | ASP R | | 36.944 | | -13.403 | 1.00 62. | | R | N |
| | MOTA | 2855 | CA | ASP R | | 36.259 | | | 1.00 61. | | R | Ĉ |
| 30 | ATOM | 2856 | CB | ASP R | | 36.043 | 14.277 | | 1.00 61. | | R | č |
| 50 | ATOM | 2857 | CG | ASP R | | 35.390 | 14.308 | -16.635 | 1.00 62. | | R | Č |
| | ATOM | 2858 | | ASP R | | 35.228 | 13.261 | -17.257 | 1.00 61. | | R | ŏ |
| | ATOM | 2859 | | ASP R | | 35.086 | | | 1.00 62. | | R | ō |
| | MOTA | 2860 | C | ASP R | | 37.139 | 12.053 | -15.616 | 1.00 60. | | R | Ċ |
| 35 | MOTA | 2861 | ō | ASP R | | 37.947 | | -16.354 | 1.00 61. | | R | Ö |
| • | ATOM | 2862 | N | ASP R | | 36.753 | 10.813 | -15.617 | 1.00 59. | 09 | R | N |
| | ATOM | 2863 | CA | ASP R | 324 | 37.332 | 9.795 | -16.458 | 1.00 59. | 54 | R | C |
| | MOTA | 2864 | CB | ASP R | | 37.447 | 8.433 | -15.700 | 1.00 58. | 18 | R | С |
| | MOTA | 2865 | CG | ASP R | 324 | 38.404 | 8.540 | | 1.00 58. | 12 | R | C |
| 40 | MOTA | 2866 | | ASP R | | 39.614 | 8.828 | | 1.00 55. | | R | 0 |
| | ATOM | 2867 | OD2 | ASP R | | 37.944 | 8.405 | -13.275 | 1.00 57. | | R | 0 |
| | MOTA | 2868 | ·C | ASP R | | 36.554 | | -17.764 | 1.00 59. | | R | C |
| | MOTA | 2869 | 0 | ASP R | | 36.891 | | -18.629 | 1.00 59. | | R | 0 |
| | MOTA. | 2870 | N | LYS R | | 35.502 | 10.483 | -17.906 | 1.00 59. | | R | N |
| 45 | ATOM | 2871 | CA | LYS R | | 34.622 | | | 1.00 58. | | R | C |
| | MOTA | 2872 | CB | LYS R | | 35.382 | | -20.361 | 1.00 59. | | R | C |
| | ATOM | 2873 | CG | LYS R | | 36.262 | | -20.325 | 1.00 63. | | R | C |
| | ATOM | 2874 | CD | LYS R | | 36.858 | | -21.703 | 1.00 65. | | R | C |
| | ATOM | 2875 | CE | LYS R | | 37.800 | | -21.724 | 1.00 68. 1.00 70. | | R | C |
| 50 | ATOM | 2876 | NZ | LYS R | | 37.884 34.087 | | -23.087 -19.095 | 1.00 70. | | R R | C N |
| | ATOM | 2877 | C | LYS R LYS R | | 33.972 | | -20.135 | 1.00 58. | | R | Õ |
| | ATOM | 2878 2879 | N O | LEU R | | 33.803 | | -17.897 | 1.00 55. | | R | N |
| | ATOM ATOM | 2880 | CA | LEU R | | 33.319 | | -17.802 | 1.00 52. | | R | C |
| 55 | ATOM | 2881 | CB | LEU R | | 33.986 | | -16.573 | 1.00 54. | | R | č |
| 33 | ATOM | 2882 | CG | LEU R | | 34.495 | | -16.818 | 1.00 55. | | R | Č |
| | ATOM | 2883 | CD1 | | | 34.879 | | -15.523 | 1.00 57. | | R | č |
| | ATOM | 2884 | CD2 | | | 33.462 | | -17.512 | 1.00 54. | | R | č |
| | ATOM | 2885 | C | LEU R | | 31.808 | 6.992 | | 1.00 50. | | R | č |
| 60 | ATOM | 2886 | Õ | LEU R | | 31.281 | | -16.536 | 1.00 48. | | R | Õ |
| 00 | ATOM | 2887 | N | TRP R | | 31.102 | 7.012 | | 1.00 47. | | R | N |
| | ATOM | 2888 | CA | TRP R | | 29.654 | | | 1.00 47. | | R | Ĉ |
| | ATOM | 2889 | CB | TRP R | | 29.148 | | -20.138 | 1.00 44. | | R | C |
| | ATOM | 2890 | CG | TRP R | | 29.596 | | -20.562 | 1.00 42. | | R | C |
| 65 | ATOM | 2891 | CD2 | | | 29.042 | | -20.137 | 1.00 40. | | R | C |
| | ATOM | 2892 | CE2 | | | 29.664 | 11.088 | -20.904 | 1.00 40. | | R | C |
| | ATOM | 2893 | CE3 | TRP R | 327 | 28.087 | | -19.188 | 1.00 38. | | R | C |
| | ATOM | 2894 | CD1 | | | 30.540 | | -21.567 | 1.00 38. | | R | C |
| | ATOM | 2895 | NE1 | . TRP R | 327 | 30.616 | 10.435 | -21.836 | 1.00 39. | 52 | R | N |

| | ATOM | 2896 | CZ2 | | | 29.329 | 12.415 -20.704 | 1.00 38.74 | R | C |
|-----|------|---------|-----|--------|-----|--------|--------------------------------|------------|---|---|
| | ATOM | 2897 | CZ3 | | | 27.747 | 11.747 -18.988 | 1.00 38.32 | R | |
| | ATOM | 2898 | CH2 | TRP F | 327 | 28.375 | 12.752 -19.752 | 1.00 39.26 | R | |
| | MOTA | 2899 | C | TRP F | 327 | 28.982 | 5.859 -18.245 | 1.00 48.40 | R | |
| 5 | ATOM | 2900 | 0 | TRP F | 327 | 29.460 | 4.746 -18.442 | 1.00 48.70 | R | |
| | ATOM | 2901 | N | SER F | 328 | 27.844 | 6.041 -17.554 | 1.00 48.50 | R | _ |
| | ATOM | 2902 | CA | SER F | | 26.995 | 4.889 -17.304 | 1.00 49.05 | R | |
| | ATOM | 2903 | CB | SER F | | 25.930 | 5.296 -16.287 | 1.00 46.82 | R | |
| | ATOM | 2904 | OG | SER F | | 24.983 | 6.165 -16.912 | 1.00 46.96 | R | |
| 10 | ATOM | 2905 | Ċ | SER F | | 26.326 | 4.464 -18.609 | 1.00 49.92 | | - |
| | ATOM | 2906 | ŏ | SER F | | 26.388 | 5.155 -19.623 | 1.00 49.92 | R | _ |
| | ATOM | 2907 | N | ASN F | | 25.712 | 3.267 -18.579 | | R | _ |
| | ATOM | 2908 | CA | ASN F | | 24.870 | 2.894 -19.704 | 1.00 49.23 | R | |
| | ATOM | 2909 | CB | ASN F | | 24.267 | 1.523 -19.395 | 1.00 48.88 | R | |
| 15 | ATOM | 2910 | CG | ASN F | | | | 1.00 49.16 | R | _ |
| 10 | ATOM | 2911 | | ASN F | | 25.347 | 0.476 -19.454 | 1.00 50.84 | R | |
| | ATOM | 2912 | | ASN F | | 26.343 | 0.615 -20.156 | 1.00 51.96 | R | |
| | ATOM | 2913 | C | | | 25.126 | -0.613 -18.698 | 1.00 49.44 | R | N |
| | | 2914 | | ASN F | | 23.743 | 3.915 -19.869 | 1.00 48.95 | R | C |
| 20 | ATOM | | 0 | ASN F | | 23.352 | 4.605 -18.938 | 1.00 48.39 | R | 0 |
| 20 | ATOM | 2915 | N | TRP F | | 23.240 | 4.032 -21.113 | 1.00 48.80 | R | N |
| | ATOM | 2916 | CA | TRP F | | 22.086 | 4.893 -21.323 | 1.00 48.88 | R | C |
| | ATOM | 2917 | CB | TRP F | | 21.711 | 4.851 -22.808 | 1.00 48.23 | R | C |
| | ATOM | 2918 | CG | TRP F | | 22.688 | 5.621 -23.615 | 1.00 47.23 | R | C |
| 0.5 | ATOM | 2919 | CD2 | | | 22.784 | 7.064 -23.719 | 1.00 47.22 | R | C |
| 25 | ATOM | 2920 | CE2 | | | 23.799 | 7.348 -24.670 | 1.00 46.29 | R | C |
| | ATOM | 2921 | CE3 | | | 22.123 | 8.119 -23.095 | 1.00 46.83 | R | C |
| | ATOM | 2922 | CD1 | | | 23.645 | 5.091 -24.508 | 1.00 47.29 | R | C |
| | ATOM | 2923 | NE1 | | | 24.333 | 6.058 -25.170 | 1.00 47.42 | R | N |
| | ATOM | 2924 | CZ2 | TRP R | 330 | 24.116 | 8.662 -24.973 | 1.00 45.44 | R | C |
| 30 | ATOM | 2925 | CZ3 | TRP R | 330 | 22.440 | 9.433 -23.398 | 1.00 46.73 | R | Č |
| | ATOM | 2926 | CH2 | TRP R | 330 | 23.448 | 9.704 -24.340 | 1.00 44.89 | R | Ċ |
| | ATOM | 2927 | С | TRP R | 330 | 20.902 | 4.414 -20.481 | 1.00 48.65 | R | č |
| | ATOM | 2928 | 0 | TRP R | 330 | 20.674 | 3.224 -20.306 | 1.00 50.55 | R | ŏ |
| | ATOM | 2929 | N | SER R | 331 | 20.152 | 5.378 -19.917 | 1.00 49.56 | R | N |
| 35 | ATOM | 2930 | CA | SER R | 331 | 18.928 | 4.997 -19.225 | 1.00 50.78 | R | Č |
| | ATOM | 2931 | CB | SER R | | 18.324 | 6.262 -18.613 | 1.00 49.15 | R | G |
| | ATOM | 2932 | OG | SER R | | 17.739 | 7.052 -19.650 | 1.00 47.98 | R | Ö |
| | ATOM | 2933 | C | SER R | | 17.935 | 4.392 -20.213 | 1.00 53.51 | | |
| | ATOM | 2934 | ō | SER R | | 18.126 | 4.413 -21.421 | 1.00 54.38 | R | C |
| 40 | ATOM | 2935 | N | GLN R | | 16.863 | 3.797 -19.663 | | R | 0 |
| | ATOM | 2936 | CA | GLN R | | 15.769 | | 1.00 55.70 | R | N |
| | ATOM | 2937 | CB | GLN R | | 14.796 | 3.410 -20.539 2.547 -19.739 | 1.00 58.54 | R | C |
| | ATOM | 2938 | CG | GLN R | | 15.428 | | 1.00 59.23 | R | C |
| | ATOM | 2939 | CD | GLN R | | | 1.227 -19.293 | 1.00 63.58 | R | C |
| 45 | ATOM | 2940 | | | | 15.638 | 0.339 -20.497 | 1.00 66.03 | R | C |
| 40 | | 2941 | OE1 | | | 14.717 | -0.152 -21.127 | 1.00 68.61 | R | 0 |
| | MOTA | | NE2 | | | 16.935 | 0.132 -20.801 | 1.00 66.39 | R | N |
| | ATOM | 2942 | C | GLN R | | 15.071 | 4.664 - 21.056 | 1.00 58.92 | R | С |
| | ATOM | 2943 | 0 | GLN R | | 15.113 | 5.728 - 20.452 | 1.00 58.59 | R | 0 |
| 50 | ATOM | 2944 | N | GLU R | | 14.454 | 4.539 - 22.238 | 1.00 59.74 | R | N |
| 50 | ATOM | 2945 | CA | GLU R | | 13.906 | 5.743 -22.834 | 1.00 61.05 | R | C |
| | MOTA | 2946 | CB | GLU R | | 13.842 | 5.582 -24.354 | 1.00 60.90 | R | C |
| | MOTA | 2947 | CG | GLU R | | 13.447 | 4.175 -24.795 | 1.00 63.18 | R | C |
| | ATOM | 2948 | CD | GLU R | | 13.527 | 4.097 -26.303 | 1.00 64.95 | R | C |
| | MOTA | 2949 | OE1 | | | 12.589 | 4.523 -26.962 | 1.00 65.07 | R | 0 |
| 55 | ATOM | 2950 | OE2 | | | 14.549 | 3.637 -26.810 | 1.00 65.85 | R | 0 |
| | MOTA | 2951 | С | GLU R | 333 | 12.531 | 6.097 -22.286 | 1.00 61.41 | R | С |
| | MOTA | 2952 | 0 | GLU R | 333 | 11.874 | 5.339 -21.585 | 1.00 62.10 | R | ŏ |
| | MOTA | 2953 | N | MET R | 334 | 12.146 | 7.340 -22.587 | 1.00 61.90 | R | N |
| | MOTA | 2954 | CA | MET R | 334 | 10.780 | 7.764 -22.370 | 1.00 63.08 | R | C |
| 60 | ATOM | 2955 | CB | MET R | | 10.672 | 8.375 -20.973 | 1.00 63.01 | R | Č |
| | MOTA | 2956 | CG | MET R | | 9.392 | 9.195 -20.797 | 1.00 63.17 | R | C |
| | ATOM | 2957 | SD | MET R | | 9.099 | 9.651 -19.083 | 1.00 65.16 | R | s |
| | ATOM | 2958 | CE | MET R | | 9.266 | 8.012 -18.359 | 1.00 62.36 | R | C |
| | ATOM | 2959 | C | MET R | | 10.413 | 8.803 -23.418 | 1.00 62.36 | | |
| 65 | ATOM | 2960 | Õ | MET R | | 11.200 | 9.678 -23.756 | 1.00 63.76 | R | C |
| | ATOM | 2961 | Ŋ | SER R | | 9.262 | 8.748 -24.104 | 1.00 63.38 | R | O |
| | ATOM | 2962 | CA | SER R | | 8.835 | 9.719 -25.151 | 1.00 64.91 | R | N |
| | ATOM | 2963 | CB | SER R | | 8.655 | 9.130 -26.526 | | R | C |
| | ATOM | 2964 | OG | SER R | | 8.514 | | 1.00 66.23 | R | C |
| | | ~ J U = | - | ~ L. I | 555 | 0.714 | 7.778 -26.432 | 1.00 68.31 | R | 0 |

| | ATOM ATOM ATOM | 2965 2966 2967 | C SER R O SER R N ILE R | 335 | 7.623 7.164 7.284 | | 4.740 3.583 5.565 | 1.00 67.14 1.00 66.71 1.00 68.37 | R R R | С О И |
|----|------------------------------|------------------------------|---|-------------------|--------------------------------------|-------------------------------------|--------------------------------------|--|------------------|------------------|
| 5 | ATOM ATOM ATOM | 2968 2969 2970 | CA ILE R CB ILE R CG2 ILE R | 336 336 | 6.234 6.666 7.733 | 13.696 -2 14.619 -2 | 5.362 4.423 5.063 4.079 | 1.00 70.69 1.00 70.06 1.00 69.34 1.00 69.89 | R R R | 0000 |
| 10 | ATOM ATOM ATOM ATOM | 2971 2972 2973 2974 | CG1 ILE R CD1 ILE R C ILE R O ILE R | 336 336 | 5.485 5.781 5.835 6.690 | 15.765 -2 | 3.018 6.728 | 1.00 69.89 1.00 69.80 1.00 73.10 1.00 73.37 | R R R | 0 0 0 |
| | ATOM ATOM ATOM | 2975 2976 2977 | N GLY R CA GLY R C GLY R | 337 337 337 | 4.574 3.906 3.582 | 14.093 -2 12.991 -2 | 8.991 | 1.00 75.30 1.00 77.98 1.00 80.70 | R R R | N C |
| 15 | ATOM ATOM ATOM ATOM | 2978 2979 2980 2981 | O GLY R N LYS R CA LYS R CB LYS R | 338 338 | 3.771 3.080 2.940 1.772 | 13.348 -3 | 1.351 | 1.00 80.91 1.00 83.73 1.00 86.40 1.00 87.18 | R R R | С И О |
| 20 | ATOM ATOM ATOM | 2982 2983 2984 | CG LYS R CD LYS R CE LYS R | 338 338 338 | 2.124 2.463 2.614 | 9.953 -3 8.709 -3 7.349 -3 | 1.819 0.943 1.841 | 1.00 88.18 1.00 89.20 1.00 90.05 | R R R | C C |
| | ATOM ATOM ATOM ATOM | 2985 2986 2987 2988 | NZ LYS R C LYS R O LYS R N LYS R | 338 338 | 3.830 3.012 3.053 3.244 | 12.883 -3 | 2.718 2.821 3.092 | 1.00 90.07 1.00 87.92 1.00 88.32 1.00 89.43 | R R R | И С О И |
| 25 | ATOM ATOM ATOM | 2989 2990 2991 | CA LYS R CB LYS R C LYS R | 339 339 | 2.989 3.608 3.687 | 11.514 -3 12.487 -3 10.064 -3 | 5.098 6.108 | 1.00 90.66 1.00 90.65 1.00 91.59 | R R R | CCC |
| 30 | ATOM ATOM ATOM | 2992 2993 2994 | O LYS R OXT LYS R CB ASP L | 339 1 | 4.948 2.966 45.108 | 9.031 -3 47.536 1 | 5.171 4.894 .9.263 | 1.00 92.23 1.00 92.68 1.00 55.28 | R R L | 0 0 0 |
| | ATOM ATOM ATOM ATOM | 2995 2996 2997 2998 | CG ASP L OD1 ASP L OD2 ASP L C ASP L | 1 1 1 | 43.772 43.684 42.739 47.516 | 46.206 2 47.833 1 | .9.777 :0.486 .9.390 | 1.00 57.07 1.00 58.59 1.00 58.03 1.00 53.88 | L L L | 0 0 0 |
| 35 | ATOM ATOM ATOM | 2999 3000 3001 | O ASP L N ASP L CA ASP L | 1 1 1 | 48.114 45.989 46.148 | 47.863 1 46.823 2 46.658 1 | .9.920 1.353 .9.903 | 1.00 53.80 1.00 54.39 1.00 53.85 | L L L | O N C |
| 40 | ATOM ATOM ATOM ATOM | 3002 3003 3004 3005 | N ILE L CA ILE L CB ILE L CG2 ILE L | 2 2 2 2 | 48.035 49.273 49.731 50.966 | 47.069 1 46.111 1 | .8.249 .7.763 .6.746 | 1.00 53.02 1.00 51.46 1.00 51.89 1.00 50.86 | L L L L | И С С |
| | ATOM ATOM ATOM | 3006 3007 3008 | CG1 ILE L CD1 ILE L C ILE L | 2 2 2 2 | 50.075 50.600 49.161 | 44.848 1 43.743 1 | .7.388 .6.271 .7.264 | 1.00 51.86 1.00 52.35 1.00 50.87 | L L L | 0 0 0 |
| 45 | MOTA MOTA ATOM | 3009 3010 3011 | O ILE L N VAL L CA VAL L | 2 3 3 | 48.216 50.048 50.093 | 49.374 1 50.795 1 | .6.492 .7.741 .7.349 | 1.00 52.29 1.00 49.99 1.00 47.23 | L L | O N C |
| 50 | ATOM ATOM ATOM ATOM | 3012 3013 3014 3015 | CB VAL L CG1 VAL L CG2 VAL L C VAL L | 3 3 3 3 | 50.385 50.543 49.243 51.288 | 53.219 1 51.541 1 | .8.564 .8.192 .9.551 .6.439 | 1.00 45.72 1.00 40.75 1.00 44.61 1.00 46.87 | L L L | C |
| | ATOM ATOM ATOM | 3016 3017 3018 | O VAL L N LEU L CA LEU L | 3 4 4 | 52.288 51.115 52.177 | 50.411 1 51.549 1 51.740 1 | .6.719 .5.306 .4.342 | 1.00 47.44 1.00 45.47 1.00 46.51 | L L | O N C |
| 55 | ATOM ATOM ATOM | 3019 3020 3021 | CB LEU L CG LEU L CD1 LEU L | 4 4 4 | 51.794 51.205 50.966 | 49.853 1 49.673 1 | .2.801 .2.683 .1.414 | 1.00 46.37 1.00 47.87 1.00 47.17 | L L | |
| 60 | MOTA MOTA MOTA MOTA | 3022 3023 3024 3025 | CD2 LEU L C LEU L O LEU L N THR L | 4 4 4 5 | 52.111 52.378 51.514 53.595 | 53.271 1 53.995 1 | .3.310 .4.306 .4.010 .4.404 | 1.00 47.09 1.00 45.92 1.00 45.62 1.00 45.95 | L L L | C 0 |
| | MOTA MOTA MOTA | 3026 3027 3028 | CA THR L CB THR L OG1 THR L | 5 5 5 | 54.023 54.812 53.831 | 55.006 1 55.199 1 54.993 1 | .4.373 .5.705 .6.770 | 1.00 46.85 1.00 46.65 1.00 47.07 | r F | C C |
| 65 | MOTA MOTA MOTA | 3029 3030 3031 | CG2 THR L C THR L O THR L | 5 5 6 | 55.159 54.846 55.915 | 55.321 1 54.893 1 | L5.835 L3.123 L3.007 | 1.00 45.76 1.00 46.19 1.00 47.94 | L L L | C 0 |
| | MOTA MOTA | 3032 3033 | N GLN L CA GLN L | 6 6 | 54.395 55.271 | | 12.249 11.051 | 1.00 45.30 1.00 44.84 | L | |

| | ATOM | 3034 | СВ | GLN L | 6 | 54.334 | 56.787 | 9.868 | 1.00 44.65 | L | С |
|----|--------------|--------------|----------|----------------|-----------------|------------------|------------------|------------------|--------------------------|---------|--------|
| | ATOM | 3035 | CG | GLN L | 6 | 53.377 | 55.566 | 9.584 | 1.00 42.77 | L | C |
| | MOTA | 3036 | CD | GLN L | 6 | 52.678 | 55.622 | 8.399 | 1.00 43.26 | Ŀ | C |
| _ | ATOM | 3037 | OE1 | GLN L | 6 | 51.527 | 55.138 | 8.442 | 1.00 40.72 | L | 0 |
| 5 | ATOM ATOM | 3038 3039 | NE2 C | GLN L GLN L | 6 6 | 53.311 56.164 | 56.196 57.684 | 7.285 11.332 | 1.00 40.31 1.00 44.60 | L L | N C |
| | ATOM | 3040 | 0 | GLN L | 6 | 55.834 | 58.708 | 12.138 | 1.00 44.62 | L | ŏ |
| | ATOM | 3041 | N | SER L | 7 | 57.360 | 57.613 | 10.803 | 1.00 44.40 | L | N |
| | ATOM | 3042 | CA | SER L | 7 | 58.136 | 58.881 | 10.869 | 1.00 44.64 | L | С |
| 10 | MOTA | 3043 | CB | SER L | 7 | 59.139 | 58.836 | 11.990 | 1.00 45.02 | Ŀ | C |
| | ATOM | 3044 | OG G | SER L | 7 | 59.810 | 57.747 | 12.082 9.567 | 1.00 43.10 1.00 44.16 | L L | 0 |
| | ATOM ATOM | 3045 3046 | C | SER L SER L | 7 7 | 58.931 59.211 | 58.984 57.952 | 9.367 | 1.00 44.16 | L | C |
| | ATOM | 3047 | N | PRO L | 8 | 59.208 | 60.157 | 9.001 | 1.00 44.18 | L | N |
| 15 | ATOM | 3048 | CD | PRO L | 8 | 59.790 | 60.409 | 7.682 | 1.00 42.55 | L | С |
| | MOTA | 3049 | CA | PRO L | 8 | 58.763 | 61.394 | 9.582 | 1.00 44.95 | Ŀ | C |
| | MOTA | 3050 | CB | PRO L | 8 | 59.465 | 62.429 | 8.780 | 1.00 45.54 | L | C |
| | ATOM ATOM | 3051 3052 | CG C | PRO L PRO L | 8 8 | 59.469 57.272 | 61.921 61.528 | 7.428 9.399 | 1.00 43.82 1.00 46.33 | L L | C |
| 20 | ATOM | 3052 | Ö | PRO L | 8 | 56.761 | 60.744 | 8.659 | 1.00 45.84 | L | ŏ |
| 20 | ATOM | 3054 | N | ALA L | 9 | 56.624 | 62.578 | 9.923 | 1.00 46.67 | L | N |
| | ATOM | 3055 | CA | ALA L | 9 | 55.199 | 62.817 | 9.692 | 1.00 47.31 | L | С |
| | MOTA | 3056 | CB | ALA L | 9 | 54.666 | 63.799 | 10.774 | 1.00 44.86 | L | C |
| 05 | MOTA | 3057 | C | ALA L | 9 | 54.997 53.994 | 63.494 63.269 | 8.291 7.637 | 1.00 47.65 1.00 47.24 | L L | C |
| 25 | ATOM ATOM | 3058 3059 | N O | ALA L SER L | 9 10 | 55.954 | 64.256 | 7.850 | 1.00 47.24 | L | N |
| | ATOM | 3060 | CA | SER L | 10 | 55.865 | 64.857 | 6.396 | 1.00 47.27 | L | C |
| | ATOM | 3061 | CB | SER L | 10 | 55.188 | 66.124 | 6.377 | 1.00 47.86 | L | C |
| | ATOM | 3062 | OG | SER L | 10 | 55.940 | 67.005 | 7.153 | 1.00 52.42 | L | 0 |
| 30 | ATOM | 3063 | C | SER L | 10 | 57.249 58.220 | 65.126 65.199 | 5.893 6.713 | 1.00 46.24 1.00 45.57 | L L | C |
| | ATOM ATOM | 3064 3065 | N O | SER L LEU L | 10 11 | 57.436 | 65.116 | 4.556 | 1.00 45.55 | L | N |
| | ATOM | 3066 | ĈA | LEU L | 11 | 58.696 | 65.349 | 4.051 | 1.00 47.02 | L | Ċ |
| | ATOM | 3067 | CB | LEU L | 11 | 59.677 | 64.273 | 4.174 | 1.00 46.19 | L | C |
| 35 | MOTA | 3068 | CG | LEU L | 11 | 59.455 | 62.842 | 3.681 | 1.00 48.73 | Ł | C |
| | MOTA | 3069 | | LEU L | 11 | 58.223 | 62.745 | 3.064 | 1.00 48.29 | L | C |
| | MOTA MOTA | 3070 3071 | CD2 C | LEU L LEU L | 11 11 | 60.627 58.582 | 62.242 65.890 | 2.868 2.664 | 1.00 47.04 1.00 47.80 | L L | C |
| | ATOM | 3071 | 0 | LEU L | 11 | 57.628 | 65.515 | 2.026 | 1.00 49.05 | L | ŏ |
| 40 | MOTA | 3073 | N | ALA L | 12 | 59.590 | 66.695 | 2.255 | 1.00 48.67 | L | N |
| | MOTA | 3074 | CA | ALA L | 12 | 59.682 | 67.388 | 0.926 | 1.00 49.18 | L | C |
| | MOTA | 3075 | CB | ALA L | 12 | 59.624 | 68.839 | 1.108 | 1.00 47.86 | L | C |
| | MOTA | 3076 3077 | C | ALA L ALA L | 12 12 | 61.038 62.069 | 66.951 66.973 | 0.353 1.136 | 1.00 49.73 1.00 50.03 | L L | C |
| 45 | ATOM ATOM | 3077 | O N | VAL L | 13 | 61.019 | 66.499 | -0.936 | 1.00 30.03 | L | И |
| 40 | ATOM | 3079 | CA | VAL L | 13 | 62.096 | 65.902 | -1.610 | 1.00 49.56 | Ŀ | Ĉ |
| | MOTA | 3080 | CB | VAL L | 13 | 61.867 | 64.417 | -1.751 | 1.00 50.10 | L | С |
| | MOTA | 3081 | | VAL L | 13 | 63.090 | 63.700 | -2.535 | 1.00 49.03 | Ŀ | C |
| 50 | MOTA | 3082 | | VAL L VAL L | 13 | 61.881 62.081 | 63.650 66.387 | -0.385 -3.096 | 1.00 48.49 1.00 49.81 | L L | C |
| 50 | ATOM ATOM | 3083 3084 | C O | VAL L | 13 13 | 60.965 | 66.532 | -3.673 | 1.00 48.90 | L | Ö |
| | MOTA | 3085 | Ň | SER L | 14 | 63.266 | 66.552 | -3.698 | 1.00 51.08 | L | N |
| | ATOM | 3086 | CA | SER L | 14 | 63.372 | 67.112 | -5.090 | 1.00 52.59 | ${f L}$ | C |
| | MOTA | 3087 | CB | SER L | 14 | 64.664 | 67.798 | -5.413 | 1.00 53.64 | L | C |
| 55 | ATOM | 3088 | OG | SER L | 14 | 65.034 63.196 | 68.809 66.058 | -4.530 -6.019 | 1.00 57.54 1.00 52.19 | L L | C |
| | ATOM ATOM | 3089 3090 | C | SER L SER L | $\frac{14}{14}$ | 63.395 | 64.859 | -5.695 | 1.00 50.20 | r L | Ö |
| | ATOM | 3091 | N | LEU L | 15 | 62.698 | 66.434 | -7.134 | 1.00 53.27 | L | N |
| | ATOM | 3092 | CA | LEU L | 15 | 62.574 | 65.390 | -8.237 | 1.00 54.53 | L | С |
| 60 | ATOM | 3093 | CB | LEU L | 15 | 62.142 | 66.024 | -9.524 | 1.00 55.40 | L | C |
| | ATOM | 3094 | CG | LEU L | 15 | 60.716 | 66.501 | -9.429 | 1.00 58.56 | Ŀ | C |
| | ATOM ATOM | 3095 3096 | | LEU L | 15 15 | 59.911 60.005 | 67.289 65.204 | -10.574 -9.238 | 1.00 58.01 1.00 60.27 | L L | C |
| | ATOM | 3096 | CD2 | LEU L | 15 | 63.914 | 64.654 | -8.459 | 1.00 55.55 | L | C |
| 65 | ATOM | 3098 | ŏ | LEU L | 15 | 64.930 | 65.289 | -8.375 | 1.00 55.36 | L | 0 |
| | ATOM | 3099 | N | GLY L | 16 | 63.795 | 63.337 | -8.663 | 1.00 56.75 | L | N |
| | ATOM | 3100 | CA | GLY L | 16 | 64.822 | 62.284 | -8.802 | 1.00 58.63 | Ŀ | C |
| | ATOM | 3101 | C | GLY L | 16 16 | 65.683 66.674 | 61.943 61.253 | -7.633 -7.795 | 1.00 60.16 1.00 61.71 | L L | C |
| | MOTA | 3102 | 0 | GLY L | ΤO | 00.0/4 | 01.200 | -1.133 | T.00 OT./I | L | J |

| | 3.000 | 2102 | NT. | CIT NT T | 17 | C 1 | E 121 | 62.607 | -6.519 | 1.00 60.61 | т | ът |
|----|-------|------|------------------|----------------|----|------------|-------|--------|--------|------------|--------|----|
| | ATOM | 3103 | N | GLN L | 17 | | 5.434 | | | | L | N |
| | ATOM | 3104 | CA | GLN L | 17 | 6. | 5.963 | 62.217 | -5.216 | 1.00 60.86 | L | C |
| | MOTA | 3105 | CB | GLN L | 17 | 6. | 5.978 | 63.455 | -4.328 | 1.00 61.98 | L | C |
| | ATOM | 3106 | ĊĠ | GLN L | 17 | _ | 6.931 | 64.635 | -4.734 | 1.00 63.16 | L | Č |
| _ | | | | | | | | | | | | |
| 5 | MOTA | 3107 | CD | GLN L | 17 | | 8.419 | 64.089 | -5.008 | 1.00 65.17 | L | C |
| | ATOM | 3108 | OE1 | GLN L | 17 | 6. | 9.148 | 63.567 | -4.073 | 1.00 65.16 | L | 0 |
| | ATOM | 3109 | NE2 | GLN L | 17 | 6 | 8.787 | 64.108 | -6.313 | 1.00 64.55 | L | N |
| | | | | | | | | | | | | |
| | MOTA | 3110 | C | GLN L | 17 | | 5.173 | 61.036 | -4.565 | 1.00 60.56 | L | С |
| | MOTA | 3111 | 0 | GLN L | 17 | 6 | 4.239 | 60.498 | -5.052 | 1.00 60.18 | L | 0 |
| 10 | ATOM | 3112 | N | ARG L | 18 | | 5.618 | 60.659 | -3.379 | 1.00 60.22 | L | N |
| 10 | | | | | | | | | | | | |
| | MOTA | 3113 | CA | ARG L | 18 | | 5.179 | 59.485 | -2.698 | 1.00 60.54 | L | C |
| | ATOM | 3114 | $^{\mathrm{CB}}$ | ARG L | 18 | 6 | 6.356 | 58.697 | -2.216 | 1.00 62.33 | L | C |
| | MOTA | 3115 | CG | ARG L | 18 | 6 | 5.975 | 57.341 | -1.777 | 1.00 66.77 | L | C |
| | | | | | | | | 56.520 | | | | |
| | ATOM | 3116 | $^{\rm CD}$ | ARG L | 18 | | 7.139 | | -1.168 | 1.00 68.42 | L | C |
| 15 | ATOM | 3117 | NE | ARG L | 18 | 6' | 7.633 | 57.422 | -0.155 | 1.00 71.65 | L | N |
| | ATOM | 3118 | CZ | ARG L | 18 | 6 | 8.200 | 57.067 | 0.931 | 1.00 73.04 | 上 | С |
| | | | | | 18 | | 8.376 | 55.781 | 1.210 | 1.00 74.42 | L | N |
| | ATOM | 3119 | NH1 | | | | | | | | | |
| | MOTA | 3120 | NH2 | ARG L | 18 | 6 | 8.597 | 58.027 | 1.771 | 1.00 73.52 | L | N |
| | MOTA | 3121 | C | ARG L | 18 | 6 | 4.423 | 59.827 | -1.432 | 1.00 59.73 | L | C |
| 20 | | 3122 | ō | ARG L | 18 | | 4.878 | 60.597 | -0.565 | 1.00 59.95 | L | 0 |
| 20 | ATOM | | | | | | | | | | | |
| | MOTA | 3123 | N | ALA L | 19 | | 3.285 | 59.225 | -1.304 | 1.00 57.66 | L | N |
| | MOTA | 3124 | CA | ALA L | 19 | 6: | 2.597 | 59.398 | -0.115 | 1.00 56.97 | L | С |
| | ATOM | 3125 | CB | ALA L | 19 | 6 | 1.261 | 59.878 | -0.465 | 1.00 56.41 | L | C |
| | | | | | | | | | | | | |
| | MOTA | 3126 | С | ALA L | 19 | | 2.473 | 58.120 | 0.563 | 1.00 56.01 | L | C |
| 25 | MOTA | 3127 | 0 | ALA L | 19 | 6 | 2.181 | 57.057 | -0.083 | 1.00 55.90 | L | 0 |
| | ATOM | 3128 | N | THR L | 20 | 6 | 2.553 | 58.230 | 1.861 | 1.00 54.57 | L | N |
| | | | | | | | | 57.145 | 2.729 | 1.00 54.71 | L | Ĉ |
| | MOTA | 3129 | $^{\mathrm{CA}}$ | THR L | 20 | | 2.530 | | | | | |
| | ATOM | 3130 | CB | THR L | 20 | 6 | 3.976 | 56.984 | 3.320 | 1.00 55.31 | L | С |
| | MOTA | 3131 | OG1 | THR L | 20 | 6 | 4.811 | 56.247 | 2.349 | 1.00 58.52 | L | О |
| 20 | | 3132 | CG2 | THR L | 20 | _ | 3.997 | 55.982 | 4.450 | 1.00 54.15 | L | C |
| 30 | ATOM | | | | | | | | | | | |
| | ATOM | 3133 | С | THR L | 20 | | 1.488 | 57.301 | 3.965 | 1.00 54.23 | L | С |
| | ATOM | 3134 | 0 | THR L | 20 | 6 | 1.495 | 58.250 | 4.662 | 1.00 55.01 | L | 0 |
| | ATOM | 3135 | N | ILE L | 21 | | 0.594 | 56.353 | 4.184 | 1.00 52.55 | L | N |
| | | | | | | | | | | | | |
| | MOTA | 3136 | CA | ILE L | 21 | | 9.478 | 56.571 | 5.138 | 1.00 51.39 | L | C |
| 35 | ATOM | 3137 | CB | ILE L | 21 | 5 | 8.267 | 56.531 | 4.332 | 1.00 51.03 | L | C |
| | ATOM | 3138 | CG2 | ILE L | 21 | | 7.101 | 56.522 | 5.229 | 1.00 50.72 | L | С |
| | | | | | | | | | | | L. | Č |
| | MOTA | 3139 | CG1 | | 21 | | 8.199 | 57.829 | 3.513 | 1.00 50.62 | | |
| | ATOM | 3140 | CD1 | ILE L | 21 | 5 | 6.828 | 57.893 | 2.664 | 1.00 51.38 | L | С |
| | ATOM | 3141 | С | ILE L | 21 | 5 | 9.550 | 55.393 | 6.102 | 1.00 50.89 | L | C |
| 40 | | 3142 | | ILE L | 21 | | 9.654 | 54.245 | 5.588 | 1.00 50.75 | L | Ö |
| 40 | ATOM | | 0 | | | | | | | | | |
| | ATOM | 3143 | N | SER L | 22 | | 9.500 | 55.604 | 7.412 | 1.00 48.72 | L | N |
| | MOTA | 3144 | CA | SER L | 22 | 5 | 9.530 | 54.455 | 8.218 | 1.00 49.28 | L | C |
| | ATOM | 3145 | СВ | SER L | 22 | | 0.870 | 54.319 | 8.753 | 1.00 50.79 | L | C |
| | | | | | | | | | | 1.00 54.83 | | |
| | MOTA | 3146 | OG | SER L | 22 | | 1.230 | 55.479 | 9.171 | | L | 0 |
| 45 | ATOM | 3147 | С | SER L | 22 | 5 | 8.395 | 54.153 | 9.139 | 1.00 48.61 | L | C |
| | ATOM | 3148 | 0 | SER L | 22 | 5 | 7.519 | 55.017 | 9.484 | 1.00 48.61 | L | 0 |
| | | | | | | | | | - | 1.00 48.09 | L | N |
| | ATOM | 3149 | N | CYS L | 23 | | 8.280 | 52.943 | 9.516 | | | |
| | ATOM | 3150 | ca | CYS L | 23 | | 7.217 | 52.634 | 10.437 | 1.00 49.40 | L | C |
| | MOTA | 3151 | С | CYS L | 23 | 5 | 7.811 | 51.946 | 11.667 | 1.00 49.17 | L | C |
| 50 | ATOM | 3152 | ŏ | CYS L | 23 | | 8.420 | 50.962 | 11.568 | 1.00 50.55 | L | 0 |
| 50 | | | | | | | | | | 1.00 47.98 | | |
| | MOTA | 3153 | CB | CYS L | 23 | | 6.230 | 51.648 | 9.696 | | L | C |
| | ATOM | 3154 | SG | CYS L | 23 | 5 | 4.576 | 51.056 | 10.342 | 1.00 52.95 | L | S |
| | ATOM | 3155 | N | LYS L | 24 | | 7.261 | 52.210 | 12.742 | 1.00 48.85 | L | N |
| | | | | | | Ē | 7.583 | | | 1.00 49.76 | | ä |
| | MOTA | 3156 | $^{\rm CA}$ | t LYS L | 24 | | | 51.323 | 14.012 | | Ŀ | C |
| 55 | MOTA | 3157 | $^{\rm CB}$ | t LYS L | 24 | 5 | 8.391 | 52.158 | 14.922 | 1.00 50.72 | Ŀ | С |
| | ATOM | 3158 | CG | LYS L | 24 | 5 | 8.429 | 51.726 | 16.593 | 1.00 52.19 | Ŀ | C |
| | | | | | 24 | | 9.897 | 51.577 | 16.954 | 1.00 55.36 | L | Ċ |
| | MOTA | 3159 | CD | LYS L | | | | | | | | _ |
| | ATOM | 3160 | CE | LYS L | 24 | | 0.182 | 50.188 | 17.675 | 1.00 56.92 | L | С |
| | MOTA | 3161 | NZ | LYS L | 24 | 6 | 1.602 | 49.679 | 17.499 | 1.00 58.53 | L | N |
| 60 | | 3162 | C | LYS L | 24 | | 6.402 | 50.795 | 14.619 | 1.00 49.31 | L | C |
| 60 | ATOM | | | | | | | | | | | |
| | ATOM | 3163 | 0 | LYS L | 24 | | 5.435 | 51.454 | 14.980 | 1.00 49.16 | L | 0 |
| | MOTA | 3164 | N | ALA L | 25 | 5 | 6.376 | 49.572 | 14.892 | 1.00 49.30 | L | N |
| | ATOM | 3165 | CA | ALA L | 25 | | 5.234 | 49.028 | 15.546 | 1.00 49.48 | L | С |
| | | | | | | | | | | | Ŀ | č |
| | ATOM | 3166 | СВ | ALA L | 25 | | 4.953 | 47.724 | 14.762 | 1.00 47.96 | | C |
| 65 | ATOM | 3167 | С | ALA L | 25 | 5 | 5.445 | 48.694 | 17.022 | 1.00 50.20 | L | С |
| | ATOM | 3168 | 0 | ALA L | 25 | | 6.480 | 48.267 | 17.399 | 1.00 49.44 | L | 0 |
| | | 3169 | | SER L | 26 | | 4.398 | 48.740 | 17.797 | 1.00 51.08 | _ L | N |
| | ATOM | | N | | | | | | | | | |
| | MOTA | 3170 | ca | SER L | 26 | | 4.567 | 48.567 | 19.242 | 1.00 53.13 | L | C |
| | MOTA | 3171 | CB | SER L | 26 | 5 | 3.332 | 49.105 | 19.920 | 1.00 52.28 | L | C |
| | | | | — - | | | | | | | | |

| | ATOM MOTA | 3172 3173 | OG C | SER L SER L | 26 26 | 52.243 54.774 | 48.435 47.175 46.923 | 19.292 19.632 20.721 | 1.00 52.65 1.00 55.40 1.00 55.86 | L L L | 0 C 0 |
|----|--------------|--------------|-----------|----------------|------------|------------------|----------------------------|----------------------------|--|-------------|-------------|
| | MOTA | 3174 3175 | O N | SER L GLU L | 26 27 | 55.013 54.637 | 46.243 | 18.729 | 1.00 56.96 | L | N |
| 5 | ATOM ATOM | 3176 | CA | GLU L | 27 | 54.838 | 44.861 | 18.928 | 1.00 57.52 | L | С |
| J | ATOM | 3177 | CB | GLU L | 27 | 53.453 | 44.334 | 19.153 | 1.00 60.89 | L | C |
| | ATOM | 3178 | CG | GLU L | 27 | 53.153 | 43.582 | 20.429 | 1.00 66.03 | L | C |
| | ATOM | 3179 | CD | GLU L | 27 | 52.824 | 44.531 | 21.585 | 1.00 70.45 | L L | 0 |
| | ATOM | 3180 | OE1 | GLU L | 27 | 51.607 | 44.914 | 21.710 22.334 | 1.00 73.02 1.00 72.02 | F F | |
| 10 | MOTA | 3181 | OE2 | GLU L | 27 | 53.793 55.191 | 44.893 44.233 | 17.624 | 1.00 56.33 | L | |
| | ATOM | 3182 | C | GLU L GLU L | 27 27 | 54.884 | 44.731 | 16.612 | 1.00 54.86 | L | |
| | ATOM | 3183 3184 | N O | SER L | 28 | 55.715 | 43.027 | 17.631 | 1.00 56.67 | L | |
| | ATOM ATOM | 3185 | CA | SER L | 28 | 56.161 | 42.382 | 16.351 | 1.00 55.27 | L | |
| 15 | ATOM | 3186 | CB | SER L | 28 | 56.723 | 41.077 | 16.656 | 1.00 53.96 | L | |
| | ATOM | 3187 | OG | SER L | 28 | 57.529 | 40.535 | 15.622 | 1.00 56.49 | Ŀ | |
| | ATOM | 3188 | C | SER L | 28 | 55.000 | 42.100 | 15.481 | 1.00 54.43 | L L | |
| | ATOM | 3189 | 0 | SER L | 28 | 54.124 | 41.630 | 15.977 14.141 | 1.00 54.12 1.00 53.99 | T. | |
| | ATOM | 3190 | N | VAL L | 29 | 55.162 54.170 | 42.207 41.736 | 13.189 | 1.00 53.99 | Ŀ | |
| 20 | ATOM | 3191 | CA | VAL L VAL L | 29 29 | 53.760 | 42.905 | 12.246 | 1.00 52.07 | L | |
| | MOTA MOTA | 3192 3193 | CB CG1 | VAL L | 29 | 53.450 | 44.030 | 13.131 | 1.00 50.61 | L | |
| | ATOM | 3194 | | VAL L | 29 | 54.794 | 43.332 | 11.216 | 1.00 50.81 | L | |
| | MOTA | 3195 | C | VAL L | 29 | 54.684 | 40.567 | 12.449 | 1.00 55.43 | Ŀ | |
| 25 | MOTA | 3196 | 0 | VAL L | 29 | 54.029 | 40.128 | 11.565 | 1.00 55.80 | L | |
| | MOTA | 3197 | N | ASP L | 30A | 55.823 | 39.964 | 12.809 | 1.00 55.85 1.00 56.24 | L L | |
| | MOTA | 3198 | CA | ASP L | 30A | 56.207 57.610 | 38.724 38.437 | 12.097 12.307 | 1.00 56.24 | L | |
| | ATOM | 3199 | CB | ASP L ASP L | 30A 30A | 58.540 | 39.376 | 11.585 | 1.00 57.40 | L | |
| 20 | MOTA MOTA | 3200 3201 | CG OD1 | ASP L | 30A | 59.709 | 39.192 | 11.915 | 1.00 63.22 | L | |
| 30 | ATOM | 3202 | | ASP L | 30A | 58.262 | 40.297 | 10.706 | 1.00 60.76 | L | |
| | ATOM | 3203 | C | ASP L | 30A | 55.441 | 37.453 | 12.548 | 1.00 55.44 | L | |
| | ATOM | 3204 | 0 | ASP L | 30A | 55.032 | 37.344 | 13.692 | 1.00 54.11 | L | |
| | MOTA | 3205 | N | ASN L | 30B | 55.172 | 36.561 | 11.637 | 1.00 56.01 | I. | |
| 35 | MOTA | 3206 | CA | ASN L | 30B | 54.376 | 35.290 | 11.874 11.102 | 1.00 56.75 1.00 57.19 | I | |
| | ATOM | 3207 | CB | ASN L | 30B | 53.122 52.338 | 35.263 33.978 | 11.310 | 1.00 57.15 | Ī | |
| | ATOM | 3208 3209 | CG OD1 | ASN L ASN L | 30B 30B | 52.062 | 33.581 | 12.461 | 1.00 56.40 | Ī | |
| | ATOM ATOM | 3210 | ND2 | | 30B | 52.051 | 33.231 | 10.119 | 1.00 56.26 | I | n N |
| 40 | MOTA | 3211 | C | ASN L | 30B | 55.197 | 34.018 | 11.810 | 1.00 57.63 | T | |
| 40 | ATOM | 3212 | ō | ASN L | 30B | 55.549 | 33.299 | 12.907 | 1.00 59.38 | I | |
| | ATOM | 3213 | N | TYR L | 30C | 55.972 | 33.851 | 10.826 | 1.00 58.12 | I | |
| | MOTA | 3214 | CA | TYR L | 30C | 56.966 | 32.728 | 11.255 10.871 | 1.00 57.56 1.00 59.59 | I | |
| | MOTA | 3215 | CB | TYR L | 30C 30C | 56.393 55.804 | 31.318 30.433 | 11.997 | 1.00 62.38 | Ī | |
| 45 | ATOM | 3216 3217 | CG CD1 | TYR L TYR L | 30C | 56.575 | 29.521 | 12.651 | 1.00 63.98 | I | |
| | ATOM ATOM | 3218 | CE1 | | 30C | 56.062 | 28.868 | 13.663 | 1.00 65.37 | I | |
| | ATOM | 3219 | CD2 | | 30C | 54.516 | 30.530 | 12.335 | 1.00 62.73 | | . Č |
| | MOTA | 3220 | CE2 | | 30C | 53.994 | | 13.359 | 1.00 65.31 | I | |
| 50 | MOTA | 3221 | CZ | TYR L | 30C | 54.751 | | 14.043 | 1.00 66.28 1.00 67.53 | I | |
| | MOTA | 3222 | OH | TYR L | 30C | 54.177 | | 15.161 10.322 | 1.00 56.78 | I | |
| | ATOM | 3223 | C | TYR L | 30C | 58.014 57.979 | | 9.221 | 1.00 56.52 | Ī | |
| | MOTA | 3224 3225 | O N | TYR L GLY L | 30C 30D | 58.707 | | 10.516 | 1.00 55.18 | I | |
| 55 | MOTA MOTA | 3226 | N CA | GLY L | 30D | 59.595 | | 9.451 | 1.00 53.84 | I | ь с |
| 55 | ATOM | 3227 | C | GLY L | 30D | 58.974 | 35.386 | 8.429 | 1.00 53.10 | | L C |
| | ATOM | 3228 | 0 | GLY L | 30D | 59.696 | | 7.594 | 1.00 52.98 | I | |
| | ATOM | 3229 | N | LYS L | 30E | 57.655 | | 8.425 | 1.00 52.44 | | L N L C |
| | MOTA | 3230 | CA | LYS L | | 57.221 | | 7.395 | 1.00 51.96 1.00 53.54 | | L C |
| 60 | ATOM | 3231 | CB | LYS L | | 56.282 56.499 | | 6.222 5.741 | 1.00 53.34 | | r C |
| | MOTA | 3232 | CG | LYS L LYS L | | 55.680 | | 6.760 | 1.00 52.44 | | r c |
| | ATOM | 3233 3234 | CD | LYS L | | 56.238 | | 6.799 | 1.00 53.21 | | ь с |
| | ATOM ATOM | 3234 | NZ | LYS L | | 55.917 | 30.965 | 7.780 | 1.00 52.68 |] | r n |
| 65 | ATOM | 3236 | Č | LYS L | | 56.619 | 37.756 | 8.105 | | | r c |
| | ATOM | 3237 | 0 | LYS L | 30E | 56.010 | | | 1.00 51.31 | | L O |
| | MOTA | 3238 | N | SER L | | 56.795 | | 7.602 | | | L N |
| | MOTA | 3239 | | | | 56.368 | | | | | r c |
| | MOTA | 3240 | СВ | SER L | 31 | 57.408 | 3 41.265 | 0.194 | T.00 #1.TO | • | |

| | 7 MOM | 2011 | OC CER I | 31 | 58.776 | 40.786 | 8.489 | 1.00 49.94 | L | 0 |
|----|--------------|--------------|---------------------|------------------|------------------|------------------|-----------------------|--------------------------|--------------|--------------|
| | ATOM ATOM | 3241 3242 | OG SER L C SER L | 31 | 55.073 | 40.596 | 7.675 | 1.00 46.30 | L | č |
| | ATOM | 3243 | O SER L | 31 | 55.007 | 40.931 | 6.496 | 1.00 47.15 | L | 0 |
| | ATOM | 3244 | N LEU L | 32 | 54.082 | 40.732 | 8.542 | 1.00 45.54 | L | N |
| 5 | MOTA | 3245 | CA LEU L | 32 | 52.707 | 40.890 | 8.042 | 1.00 44.95 | <u>r</u> | C |
| | MOTA | 3246 | CB LEU L | 32 | 51.658 | 40.126 | 8.959 | 1.00 43.45 | Ľ | C |
| | MOTA | 3247 | CG LEU L | 32 | 51.951 | 38.635 | 9.078 | 1.00 42.44 | L L | C |
| | MOTA | 3248 | CD1 LEU L | 32 | 50.943 | 37.801 | 9.742 | 1.00 40.43 1.00 40.35 | L | C |
| | ATOM | 3249 | CD2 LEU L | 32 | 52.063 52.494 | 38.084 42.421 | 7.588 8.128 | 1.00 40.33 | L | G |
| 10 | MOTA | 3250 | C LEU L | 32 32 | 51.620 | 42.421 | 8.861 | 1.00 45.96 | L | ŏ |
| | ATOM ATOM | 3251 3252 | O LEU L N MET L | 33 | 53.135 | 43.182 | 7.215 | 1.00 44.68 | L | N |
| | ATOM | 3253 | CA MET L | 33 | 53.114 | 44.629 | 7.195 | 1.00 46.62 | L | C |
| | ATOM | 3254 | CB MET L | 33 | 54.453 | 45.212 | 7.636 | 1.00 48.40 | L | С |
| 15 | ATOM | 3255 | CG MET L | 33 | 54.706 | 46.723 | 7.347 | 1.00 51.53 | L | C |
| | MOTA | 3256 | SD MET L | 33 | 53.565 | 47.476 | 8.816 | 1.00 57.60 | L | S |
| | MOTA | 3257 | CE MET L | 33 | 54.234 | 47.188 | 10.430 | 1.00 55.27 | ŗ | C |
| | MOTA | 3258 | C MET L | 33 | 52.978 | 44.924 | 5.655 | 1.00 45.90 | L | C |
| | ATOM | 3259 | O MET L | 33 | 53.599 | 44.269 | $\frac{4.780}{5.33}$ | 1.00 45.80 1.00 43.80 | L L | N |
| 20 | ATOM | 3260 | N HIS L | 34 | 52.113 51.930 | 45.875 46.321 | 5.332 3.910 | 1.00 43.80 | L | C |
| | MOTA | 3261 | CA HIS L | 34 34 | 50.514 | 45.888 | 3.633 | $1.00 \ 42.70$ | Ĺ | č |
| | ATOM ATOM | 3262 3263 | CB HIS L | 34 | 50.190 | 44.505 | 4.049 | 1.00 41.65 | Ľ | Ċ |
| | ATOM | 3264 | CD2 HIS L | 34 | 49.217 | 44.047 | 4.864 | 1.00 44.21 | L | С |
| 25 | ATOM | 3265 | ND1 HIS L | 34 | 50.838 | 43.400 | 3.574 | 1.00 42.76 | L | N |
| | ATOM | 3266 | CE1 HIS L | 34 | 50.297 | 42.330 | 4.140 | 1.00 43.50 | ${f L}$ | С |
| | MOTA | 3267 | NE2 HIS L | 34 | 49.304 | 42.711 | 4.907 | 1.00 42.79 | Ŀ | N |
| | ATOM | 3268 | C HIS L | 34 | 51.890 | 47.798 | 3.859 | 1.00 42.81 | Ŀ | C |
| | MOTA | 3269 | O HIS L | 34 | 51.722 | 48.488 | 4.923 | 1.00 44.23 | L | O NT |
| 30 | MOTA | 3270 | N TRP L | 35 | 52.117 | 48.370 | 2.676 | 1.00 41.84 1.00 41.57 | , L L | N C |
| | ATOM | 3271 | CA TRP L | 35 | 52.202 53.559 | 49.815 50.142 | $2.481 \\ 2.025$ | 1.00 41.37 | L | C |
| | ATOM | 3272 | CB TRP L | 35 35 | 54.525 | 50.142 | 3.172 | 1.00 40.40 | L | č |
| | ATOM ATOM | 3273 3274 | CG TRP L | 35 35 | 54.944 | 51.224 | 3.971 | 1.00 41.73 | Ľ | Č |
| 35 | ATOM | 3275 | CE2 TRP L | 35 | 56.052 | 50.760 | 4.800 | 1.00 41.68 | L | C |
| 33 | MOTA | 3275 | CE3 TRP L | 35 | 54.491 | 52.502 | 4.165 | 1.00 40.10 | L | C |
| | ATOM | 3277 | CD1 TRP L | 35 | 55.573 | 49.170 | 3.306 | 1.00 41.34 | L | C |
| | ATOM | 3278 | NE1 TRP L | 35 | 56.439 | 49.548 | 4.300 | 1.00 41.83 | L | \mathbf{N} |
| | MOTA | 3279 | CZ2 TRP L | 35 | 56.704 | 51.592 | 5.736 | 1.00 41.45 | Ŀ | Ç |
| 40 | ATOM | 3280 | CZ3 TRP L | 35 | 55.082 | 53.332 | 5.309 | 1.00 41.11 | L | C |
| | MOTA | 3281 | CH2 TRP L | 35 | 56.169 | 52.825 | 6.002 | 1.00 41.44 | L | C |
| | MOTA | 3282 | C TRP L | 35 | 51.210 | 50.279 | $1.457 \\ 0.372$ | 1.00 42.23 1.00 43.53 | L L | C |
| | MOTA | 3283 | O TRP L | 35 | 51.012 50.489 | 49.567 51.384 | $\frac{0.372}{1.725}$ | 1.00 40.06 | L | N |
| 45 | MOTA | 3284 3285 | N TYR L CA TYR L | 36 36 | 49.548 | 51.881 | 0.769 | 1.00 39.58 | Ĺ | Ĉ |
| 45 | ATOM ATOM | 3286 | CB TYR L | 36 | 48.068 | 51.823 | 1.298 | 1.00 38.10 | L | Ċ |
| | ATOM | 3287 | CG TYR L | 36 | 47.633 | 50.524 | 1.872 | 1.00 39.65 | ${f L}$ | C |
| | ATOM | 3288 | CD1 TYR L | 36 | 48.018 | 50.099 | 3.040 | 1.00 37.47 | L | C |
| | MOTA | 3289 | CE1 TYR L | 36 | 47.728 | 48.721 | 3.438 | 1.00 37.52 | L | C |
| 50 | MOTA | 3290 | CD2 TYR L | 36 | 47.005 | 49.647 | 1.020 | 1.00 36.92 | \mathbf{L} | C |
| | ATOM | 3291 | CE2 TYR L | 36 | 46.662 | 48.284 | 1.426 | 1.00 36.87 | Ŀ | C |
| | MOTA | 3292 | CZ TYR L | 36 | 47.070 | 47.850 | 2.651 | 1.00 37.75 | Ŀ | C |
| | MOTA | 3293 | OH TYR L | 36 | 46.782 | 46.544 | 3.043 | 1.00 39.29 1.00 40.31 | L L | O C |
| | ATOM | 3294 | C TYR L | 36 36 | 49.883 | 53.400 54.086 | 0.509 1.359 | 1.00 40.31 | L | ŏ |
| 55 | MOTA | 3295 | O TYR L N GLN L | 36 37 | 50.509 49.535 | 53.818 | -0.725 | 1.00 39.96 | L | Ŋ |
| | MOTA MOTA | 3296 3297 | N GLN L CA GLN L | 3 <i>7</i> 37 | 49.704 | 55.158 | -1.255 | 1.00 40.83 | L | Ċ |
| | ATOM | 3298 | CB GLN L | 37 | 50.186 | 55.133 | -2.658 | 1.00 39.79 | L | C |
| | MOTA | 3299 | CG GLN L | 37 | 50.494 | 56.431 | -3.274 | 1.00 42.07 | L | С |
| 60 | MOTA | 3300 | CD GLN L | | 51.024 | 56.484 | -4.754 | 1.00 44.50 | ${f L}$ | С |
| • | ATOM | 3301 | OE1 GLN L | 37 | 50.377 | 56.066 | -5.645 | 1.00 47.36 | L | 0 |
| | MOTA | 3302 | NE2 GLN L | | 52.180 | 57.013 | -4.930 | 1.00 43.45 | L | N |
| | MOTA | 3303 | C GLN L | 37 | 48.324 | 55.765 | -1.490 | 1.00 40.88 | Ŀ | C |
| | MOTA | 3304 | O GLN L | | 47.497 | 55.064 | -2.111 | 1.00 39.82 | L T. | O |
| 65 | MOTA | 3305 | N GLN L | | 48.031 | 56.962 | -0.927 | 1.00 41.63 1.00 42.50 | L L | N C |
| | ATOM | 3306 | CA GLN L | | 46.767 | 57.644 57.803 | -1.200 0.033 | 1.00 42.30 | r L | C |
| | MOTA | 3307 | CB GLN L | | 45.989 44.570 | 58.433 | -0.190 | 1.00 42.20 | L | C |
| | ATOM ATOM | 3308 3309 | CG GLN L | | 43.661 | 58.451 | 1.068 | 1.00 42.42 | Ĺ | č |
| | AT OH | 5505 | لل ۱۱۰۰ می | 50 | | | | | | |

| | ATOM | 3310 | OE1 GL | N L | 38 | 44.153 | 58.584 | 2.191 | 1.00 40.92 | L | 0 |
|-----|--------------|--------------|--------|----------------|----------|------------------|------------------|------------------|--------------------------|--------------|--------|
| | ATOM | | | | 38 | 42.275 | 58.205 | 0.809 | 1.00 41.03 | <u>r</u> | N |
| | ATOM | | | N L | 38 | 47.132 | 59.057 | -1.704 | 1.00 43.48 | <u> </u> | C |
| | ATOM | | | N L | 38 | 47.433 | 59.962 | -0.961 | 1.00 43.75 | L | O |
| 5 | ATOM | 3314 | N LY | S L | 39 | 47.003 | 59.229 | -2.988 | 1.00 45.16 | L L | C N |
| • | ATOM | 3315 | | ZS L | 39 | 47.000 | 60.502 | -3.632 | 1.00 46.88 | L | C |
| | ATOM | 3316 | | KS L | 39 | 47.079 | 60.354 | -5.121 | 1.00 48.09 1.00 50.07 | L L | Ċ |
| | ATOM | - | | ZS L | 39 | 48.104 | 59.370 | -5.531 -6.952 | 1.00 53.52 | L | č |
| | MOTA | | | KS L | 39 | 48.627 | 59.508 58.426 | -7.919 | 1.00 56.25 | L | Č |
| 10 | ATOM | | | YS L | 39 | 48.304 | 58.420 | -8.719 | 1.00 56.24 | L | N |
| | ATOM | | | YS L | 39 | 49.534 45.820 | 61.324 | -3.269 | 1.00 47.86 | L | C |
| | MOTA | | | YS L | 39 | 44.811 | 60.782 | -2.807 | 1.00 47.17 | L | 0 |
| | ATOM | | | YS L | 39 | 45.967 | 62.651 | -3.375 | 1.00 48.23 | L | N |
| | MOTA | | | RO L | 40 40 | 47.119 | 63.387 | -3.934 | 1.00 48.78 | L | С |
| 15 | ATOM | | | RO L | 40 | 44.892 | 63.548 | -3.036 | 1.00 48.38 | L | C |
| | MOTA | | | RO L · RO L | 40 | 45.487 | 64.858 | -3.472 | 1.00 49.68 | L | С |
| | ATOM | | | RO L | 40 | 46.955 | 64.694 | -3.202 | 1.00 50.16 | \mathbf{L} | C |
| | ATOM | | | RO L | 40 | 43.592 | 63.400 | -3.829 | 1.00 48.85 | L | C |
| 00 | ATOM ATOM | 3329 | - | RO L | 40 | 43.605 | 63.329 | -5.042 | 1.00 48.79 | L | 0 |
| 20 | ATOM | | | LY L | 41 | 42.472 | 63.239 | -3.114 | 1.00 49.59 | Г | N |
| | ATOM | 3331 | | LYL | 41 | 41.156 | 62.982 | -3.786 | 1.00 50.02 | L | C |
| | ATOM | 3332 | | LY L | 41 | 40.830 | 61.537 | -4.182 | 1.00 50.71 | L | C |
| | ATOM | 3333 | - | LY L | 41 | 39.765 | 61.195 | -4.532 | 1.00 50.67 | L | 0 |
| 25 | ATOM | 3334 | - | LN L | 42 | 41.824 | 60.716 | -4.258 | 1.00 50.87 | Ŀ | N |
| 20 | ATOM | 3335 | | LN L | 42 | 41.796 | 59.300 | -4.507 | 1.00 51.75 | L | C |
| | ATOM | 3336 | | LN L | 42 | 43.039 | 59.072 | -5.281 | 1.00 52.91 | L | C |
| • | ATOM | 3337 | | LN L | 42 | 42.948 | 59.658 | -6.822 | 1.00 55.22 | Ţ | C |
| | ATOM | 3338 | CD G | LN L | 42 | 44.150 | 59.256 | -7.607 | 1.00 56.68 | L | 0 |
| 30 | ATOM | 3339 | OE1 G | LN L | 42 | 44.755 | 60.170 | -8.261 | 1.00 58.21 | L L | И |
| | MOTA | 3340 | NE2 G | LN L | 42 | 44.623 | 57.918 | -7.519 | 1.00 57.44 | r L | C |
| 131 | ATOM | 3341 | C G | LN L | 42 | 41.764 | 58.317 | -3.141 | 1.00 50.97 1.00 51.08 | L | Ö |
| | MOTA | 3342 | | LN L | 42 | 41.808 | 58.707 | -2.045 | 1.00 51.08 | L | N |
| | MOTA | 3343 | | ER L | 43 | 41.523 | 57.062 | -3.326 | 1.00 49.33 | L | Č |
| 35 | MOTA | 3344 | | ER L | 43 | 41.337 | 56.114 | -2.324 -2.712 | 1.00 50.00 | L L | č |
| | MOTA | 3345 | | ER L | 43 | 40.209 | 55.257 54.393 | -3.771 | 1.00 52.62 | L | ó |
| | ATOM | 3346 | | ER L | 43 | 40.679 | | -2.199 | 1.00 46.70 | L | č |
| | MOTA | 3347 | | SER L | 43 | 42.800 | 55.404 55.641 | -3.047 | 1.00 45.07 | L | Ö |
| | ATOM | 3348 | | SER L | 43 | 43.674 | 54.829 | -1.039 | 1.00 46.29 | L | N |
| 40 | MOTA | 3349 | | PRO L | 44 | 43.118 42.200 | 54.695 | 0.070 | 1.00 47.19 | L | |
| | MOTA | 3350 | | PRO L | 44 | 44.345 | 54.129 | -0.843 | 1.00 46.37 | L | |
| | MOTA | 3351 | | PRO L | 44 | 44.180 | 53.413 | 0.387 | 1.00 46.52 | L | |
| | MOTA | 3352 | | PRO L | 44 | 43.084 | 54.301 | 1.176 | 1.00 47.07 | L | C |
| | ATOM | 3353 | | PRO L | 44 | 44.586 | 53.048 | -1.945 | 1.00 46.83 | L | |
| 45 | MOTA | 3354 | | PRO L | 44 | 43.649 | 52.520 | -2.368 | 1.00 47.16 | L | O |
| | MOTA | 3355 | | | 45 | 45.807 | | -2.306 | 1.00 46.19 | L | |
| | ATOM | 3356 3357 | | LYS L | 45 | 46.236 | 51.816 | -3.267 | 1.00 47.13 | L | |
| | ATOM ATOM | 3358 | | LYS L | 45 | 46.560 | | -4.574 | 1.00 46.21 | L | |
| EO | ATOM | 3359 | | LYS L | 45 | 47.534 | | -5.593 | 1.00 49.79 | L | |
| 50 | MOTA | 3360 | | LYS L | 45 | 47.328 | | -7.044 | 1.00 53.61 | I | |
| | ATOM | 3361 | | LYS L | 45 | 48.384 | | -8.178 | 1.00 55.08 | I | |
| | MOTA | 3362 | | LYS L | 45 | 48.007 | 51.167 | -9.072 | 1.00 59.14 | Ī | |
| | MOTA | 3363 | | LYS L | 45 | 47.439 | | -2.780 | 1.00 46.15 | I | |
| 55 | MOTA | 3364 | | LYS L | 45 | 48.367 | 51.601 | -2.208 | | Ī | |
| 55 | MOTA | 3365 | | LEU L | 46 | 47.439 | | -3.087 | | I | |
| | MOTA | 3366 | | LEU L | 46 | 48.420 | 48.871 | | | Ī | |
| | MOTA | 3367 | | LEU L | 46 | 47.967 | | | | I | |
| | ATOM | 3368 | | LEU L | 46 | 49.091 | 46.349 | | | I | |
| 60 | ATOM | 3369 | | LEU L | 46 | 49.245 | 46.386 | | | I | |
| 50 | MOTA | 3370 | | LEU L | 46 | 48.519 | 44.936 | | 1.00 43.61 | I | |
| | ATOM | 3371 | | LEU L | 46 | 49.719 | 48.986 | | | I | |
| | MOTA | | | LEU L | | 49.784 | | | | | |
| | MOTA | | | LEU L | | 50.822 | 49.188 | -2.491 | 1.00 43.91 | | |
| 65 | ATOM | | | LEU L | | 52.11 | | | | I | |
| 00 | ATOM | | | LEU L | | 52.82 | | | | 1 | i C |
| | ATOM | | CG | LEU L | 47 | 52.34 | | -2.865 | 1.00 45.79 | | r C |
| | ATOM | | CD1 | LEU L | 47 | 53.21 | | | 1.00 43.54 | | r C |
| | ATOM | | | LEU L | 47 | 52.64 | 5 52.217 | -4.259 | 1.00 44.99 | J | r C |
| | | | | | | | | | | | |

| | | | | | | | | 1.00 43.22 | L | С |
|------|--------------|--------------|------------------------|--------------|------------------|------------------|----------------------|--------------------------|--------------|--------------|
| | ATOM | 3379 | C LEU L | 47 47 | 52.920 53.660 | | -3.804 | 1.00 43.02 | L | 0 |
| | MOTA MOTA | 3381 1 | M ILE L | 48 | 53.024 | 47.708 46.659 | -1.562 -1.077 | 1.00 42.64 1.00 44.20 | L L | N C |
| 5 | MOTA MOTA | | CA ILE L CB ILE L | 48 48 | 53.893 55.148 | 47.296 | -0.472 | 1.00 44.06 1.00 42.39 | L L | C |
| 5 | MOTA | 3384 (| CG2 ILE L | 48 48 | 56.083 55.895 | 46.170 48.103 | -1.540 | 1.00 43.43 | L | С |
| | ATOM ATOM | | CD1 ILE L | 48 | 57.123 | 47.375 45.824 | -2.060 -0.013 | 1.00 45.86 1.00 44.86 | L L | C |
| 10 | ATOM ATOM | | O ILE L | 48 48 | 53.169 52.713 | 46.305 | 0.993 | 1.00 44.44 | r F | N |
| 10 | MOTA | 3389 | N TYR L | 49 49 | 53.069 52.544 | 44.523 43.575 | -0.336 0.646 | 1.00 43.51 1.00 44.25 | L | С |
| | MOTA MOTA | | CA TYR L CB TYR L | 49 | 51.447 | 42.725 | -0.007 -1.095 | 1.00 44.43 1.00 47.66 | L L | C |
| 4.00 | MOTA | 3392 | CG TYR L CD1 TYR L | 49 49 | 51.998 52.302 | 41.866 40.531 | -0.831 | 1.00 48.71 | L | С |
| 15 | MOTA ATOM | 3394 | CE1 TYR L | 49 | 52.574 51.996 | 39.656 42.319 | -1.873 -2.415 | 1.00 48.62 1.00 46.74 | L L | C |
| | ATOM ATOM | | CD2 TYR L CE2 TYR L | 49 49 | 52.278 | 41.447 | -3.456 | 1.00 47.16 | L | C |
| | MOTA | 3397 | CZ TYR L | 49 49 | 52.567 52.841 | 40.122 39.246 | -3.189 -4.221 | 1.00 47.68 1.00 49.06 | L | 0 |
| 20 | ATOM ATOM | 3398 3399 | C TYR L | 49 | 53.626 | 42.684 | 1.269 0.719 | 1.00 44.97 1.00 44.07 | L L | C |
| | MOTA | 3400 | O TYR L N ARG L | 49 50 | 54.695 53.318 | 42.452 42.219 | 2.485 | 1.00 44.80 | L | N |
| | MOTA MOTA | 3401 3402 | CA ARG L | . 50 | 54.318 | 41.356 | 3.209 2.609 | 1.00 46.52 1.00 47.86 | L L | C |
| 25 | ATOM | 3403 3404 | CB ARG L | 50 50 | 54.263 54.273 | 39.963 38.890 | 3.685 | 1.00 49.22 | : L | C |
| | MOTA MOTA | 3405 | CD ARG L | 50 | 54.342 53.536 | 37.481 37.403 | 3.085 1.865 | 1.00 49.53 1.00 51.67 | | N |
| | MOTA MOTA | 3406 3407 | NE ARG L CZ ARG L | 50 50 | 53.801 | 36.394 | 1.017 | 1.00 52.68 1.00 53.20 | B L | C N |
| 30 | MOTA | 3408 | NH1 ARG L | 50 50 | 54.765 53.036 | 35.533 36.226 | 1.290 -0.066 | 1.00 52.22 | 2 L | N |
| | MOTA MOTA | 3409 3410 | NH2 ARG L C ARG L | 50 | 55.780 | 41.844 | 3.283 3.136 | 1.00 46.28 | B L L L | C O |
| | MOTA | 3411 | O ARG L N ALA L | 50 51 | 56.760 55.831 | 41.090 43.166 | 3.535 | 1.00 45.86 | 5 L | N |
| 35 | MOTA MOTA | 3412 3413 | CA ALA L | 51 | 56.996 | 44.060 43.478 | 3.797 4.954 | 1.00 44.82 1.00 45.10 | 2 L | C |
| | MOTA MOTA | 3414 3415 | CB ALA L | 51 51 | 57.806 58.054 | 44.322 | 2.684 | 1.00 46.1 | 4 L | C |
| | ATOM | 3416 | O ALA L | 51 | 58.836 58.146 | 45.259 43.438 | 2.765 1.650 | 1.00 47.3 1.00 44.6 | | N |
| 40 | ATOM ATOM | 3417 3418 | N SER L | 52 52 | 59.178 | 43.624 | 0.583 | 1.00 45.9 1.00 42.7 | | C |
| 40 | MOTA | 3419 | CB SER L | | 60.482 60.249 | 42.894 41.539 | 0.955 1.329 | 1.00 43.6 | 2 L | 0 |
| | MOTA ATOM | 3420 3421 | C SER L | 52 | 58.718 | 43.186 | -0.849 -1.810 | 1.00 47.1 1.00 48.3 | 9 L 8 L | C 0 |
| 4.5 | MOTA | 3422 3423 | O SER L N ASN L | | 59.467 57.403 | 43.297 42.790 | -0.932 | 1.00 49.2 | 0 F | N |
| 45 | MOTA MOTA | 3424 | CA ASN L | 53 | 56.750 55.792 | | | 1.00 51.2 1.00 52.8 | 6 L 0 L | |
| | MOTA MOTA | 3425 3426 | CB ASN I | | 56.547 | 39.817 | -1.926 | 1.00 55.5 | 8 L | |
| | MOTA | 3427 | OD1 ASN I | 53 | 57.180 56.499 | | | 1.00 55.7 | '9 L | \mathbf{N} |
| 50 | MOTA MOTA | 3428 3429 | ND2 ASN I C ASN I | 53 ر | 55.998 | 43.325 | -2.976 | 1.00 51.9 | 0 L | |
| | MOTA | 3430 | O ASN I | | 54.932 56.626 | | | 1.00 52.0 |)1 L | N |
| | MOTA MOTA | | CA LEU I | 54 | 56.044 | 44.648 | -5.060 | | 38 I 15 I | C |
| 55 | ATOM | | CB LEU I | | 57.080 56.676 | 5 46.173 | -7.022 | 1.00 54.4 | 16 I | , C |
| | MOTA MOTA | 3435 | CD1 LEU I | ւ 54 | 56.434 57.738 | | | |)9 I 24 I | , C |
| | MOTA ATOM | | | ն 54 ն 54 | 54.749 | 9 44.151 | L -5.720 | 1.00 53. | 72 I | |
| 60 | MOTA | 3438 | O LEU | ւ 54 | 54.703 53.62 | | | 1.00 53. | 51 I | N |
| | MOTA MOTA | | | ւ 55 | 52.36 | 8 44.478 | 8 -6.116 | 5 1.00 55. | 11 I | |
| | ATOM | 3441 | . CB GLU | ь 55 | 51.29 49.97 | | 4 -5.592 5 -6.300 | 1.00 55. | 64 I | . C |
| 65 | ATOM ATOM | | CD GLU | ь 55 | 49.16 | 9 43.96 | 9 -5.835 | 5 1.00 57. | 19 I 60 I | . O |
| 00 | ATOM | 3444 | OE1 GLU | ь 55 ь 55 | 49.76 47.88 | | | 2 1.00 56. | 57 | <u>ن</u> 0 |
| | ATOM ATOM | | C GLU | L 55 | 52.36 | 0 44.66 | 2 -7.650 | 0 1.00 55. | | L C |
| | ATOM | | 7 O GLU | ь 55 | 52.87 228 | 0 45.53 | Z -0.21 | , <u>1.00 55.</u> | | |
| | | | | | | | | | | |

| | ATOM | 3448 | N | SER L | 56 | 51.750 | 43.781 | -8.303 | 1.00 56.80 | I | ı N |
|-----|--------------|--------------|--------------|----------------|-----------|------------------|------------------|------------------|--------------------------|--------|-----|
| | ATOM | 3449 | CA | SER L | 56 | 51.755 | 43.837 | -9.703 | 1.00 58.42 | L | |
| | ATOM | 3450 | CB | SER L | 56 | 50.933 | 42.610 | -10.158 | 1.00 58.40 | I | _ |
| _ | ATOM | 3451 | OG | SER L | 56 | 50.926 | 42.846 | -11.533 | 1.00 62.54 | L | |
| 5 | ATOM | 3452 | C | SER L | 56 | 51.163 | 45.190 | -10.225 | 1.00 57.30 | L | _ |
| | MOTA | 3453 | 0 | SER L | 56 | 50.186 | 45.761 | -9.731 | 1.00 57.56 | Ī | _ |
| | ATOM | 3454 | N | GLY L | 57 | 51.874 | 45.796 | -11.127 | 1.00 57.37 | L | |
| | MOTA | 3455 | CA | GLY L | 57 57 | 51.424 | 47.049 | -11.688 | 1.00 56.96 | L | - |
| 40 | MOTA | 3456 | C | GLY L | 57 | 52.204 | 48.193 | -11.119 | 1.00 56.79 | L | |
| 10 | ATOM ATOM | 3457 3458 | O | GLY L ILE L | 57 58 | 52.157 52.895 | 49.231 | -11.753 | 1.00 58.79 1.00 55.41 | L | _ |
| | ATOM | 3459 | N CA | ILE P | 58 | 53.508 | 48.026 49.177 | -9.960 -9.257 | 1.00 53.41 | I. | |
| | ATOM | 3460 | CB | ILE L | 58 | 53.534 | 48.875 | -7.833 | 1.00 53.96 | L | |
| | ATOM | 3461 | CG2 | ILE L | 58 | 54.205 | 49.855 | -7.156 | 1.00 51.43 | L | |
| 15 | ATOM | 3462 | CG1 | | 58 | 52.121 | 48.769 | -7.308 | 1.00 50.04 | ī | |
| | MOTA | 3463 | CD1 | | 58 | 51.212 | 50.082 | -7.601 | 1.00 50.72 | ī | |
| | ATOM | 3464 | C | ILE L | 58 | 54.878 | 49.294 | -9.751 | 1.00 54.15 | ī | |
| | ATOM | 3465 | Ō | ILE L | 58 | 55.493 | 48.283 | -9.888 | 1.00 55.21 | Ī | |
| | ATOM | 3466 | N | PRO L | 59 | 55.399 | 50.473 | -10.051 | 1.00 53.53 | L | |
| 20 | ATOM | 3467 | CD | PRO L | 59 | 54.706 | 51.752 | -10.212 | 1.00 52.32 | L | |
| | ATOM | 3468 | CA | PRO L | 59 | 56.800 | 50.603 | -10.428 | 1.00 53.60 | L | C |
| | ATOM | 3469 | CB | PRO L | 59 | 56.943 | 52.058 | -10.742 | 1.00 51.95 | L | C |
| | MOTA | 3470 | CG | PRO L | 59 | 55.586 | 52.664 | -10.254 | 1.00 51.28 | L | |
| | MOTA | 3471 | C | PRO L | 59 | 57.867 | 50.269 | -9.460 | 1.00 54.47 | I | |
| 25 | ATOM | 3472 | 0 | PRO L | 59 | 57.709 | 50.423 | -8.128 | 1.00 55.96 | L | |
| | ATOM | 3473 | N | ALA L | 60 | 58.970 | 49.767 | -10.063 | 1.00 54.31 | L | |
| | MOTA | 3474 | CA | ALA L | 60 | 60.165 | 49.330 | -9.309 | 1.00 54.02 | L | |
| | ATOM | 3475 3476 | CB | ALA L | 60 | 61.266 | 48.623 50.494 | -10.235 | 1.00 53.41 | L | |
| 30 | ATOM ATOM | 3477 | С 0 | ALA L ALA L | ·60 60 | 60.854 61.789 | 50.494 | -8.512 -7.714 | 1.00 53.88 1.00 53.56 | L | |
| 30 | ATOM | 3477 | N | ARG L | 61 | 60.503 | 51.752 | -8.815 | 1.00 53.36 | L L | |
| | ATOM | 3479 | CA | ARG L | 61 | 60.979 | 52.803 | -7.943 | 1.00 53.40 | L | - |
| | ATOM | 3480 | CB | ARG L | 61 | 60.491 | 54.163 | -8.394 | 1.00 54.39 | L | |
| | ATOM | 3481 | CG | ARG L | 61 | 60.284 | 54.239 | -9.802 | 1.00 55.57 | L | |
| 35 | ATOM | 3482 | CD | ARG L | 61 | 59.850 | 55.654 | -10.234 | 1.00 58.75 | L | |
| | ATOM | 3483 | NE | ARG L | 61 | 58.422 | 55.955 | -10.333 | 1.00 60.43 | L | |
| | MOTA | 3484 | CZ | ARG L | 61 | 57.733 | 56.569 | -9.387 | 1.00 61.42 | L | |
| | MOTA | 3485 | NH1 | ARG L | 61 | 58.344 | 56.916 | -8.329 | 1.00 61.49 | L | |
| | ATOM | 3486 | NH2 | ARG L | 61 | 56.475 | 56.905 | -9.543 | 1.00 60.78 | L | N |
| 40 | MOTA | 3487 | С | ARG L | 61 | 60.565 | 52.561 | -6.456 | 1.00 51.50 | L | C |
| | ATOM | 3488 | 0 | ARG L | 61 | 61.109 | 53.120 | -5.595 | 1.00 51.57 | L | |
| | ATOM | 3489 | N | PHE L | 62 | 59.529 | 51.811 | -6.212 | 1.00 50.00 | L | |
| | MOTA | 3490 | CA | PHE L | 62 | 59.032 | 51.632 | -4.935 | 1.00 49.93 | L | _ |
| 45 | ATOM | 3491 | CB | PHE L | 62 | 57.467 | 51.469 | -4.961 | 1.00 47.93 | L | |
| 45 | MOTA | 3492 3493 | CG CD1 | PHE L | 62 | 56.737 | 52.754 | -5.178 | 1.00 48.92 | L | |
| | ATOM ATOM | 3494 | | PHE L | 62 62 | 56.522 56.365 | 53.651 53.122 | -4.150 -6.376 | 1.00 48.20 1.00 48.67 | L L | |
| | ATOM | 3495 | | PHE L | 62 | 55.873 | 54.853 | -4.358 | 1.00 48.82 | L | |
| | ATOM | 3496 | CE2 | | 62 | 55.859 | 54.350 | -6.619 | 1.00 49.21 | L | |
| 50 | MOTA | 3497 | CZ | PHE L | 62 | 55.528 | 55.210 | -5.657 | 1.00 47.07 | L | |
| | ATOM | 3498 | Č | PHE L | 62 | 59.627 | 50.305 | -4.485 | 1.00 50.05 | L | |
| | ATOM | 3499 | Ó | PHE L | 62 | 59.369 | 49.281 | -5.181 | 1.00 51.12 | L | |
| | ATOM | 3500 | N | SER L | 63 | 60.115 | 50.244 | -3.287 | 1.00 48.79 | L | |
| | ATOM | 3501 | CA | SER L | 63 | 60.627 | 49.031 | -2.616 | 1.00 49.33 | L | |
| 55 | MOTA | 3502 | CB | SER L | 63 | 62.221 | 48.902 | -2.650 | 1.00 48.44 | L | |
| | MOTA | 3503 | OG | SER L | 63 | 62.867 | 50.204 | -2.559 | 1.00 52.96 | L | 0 |
| | MOTA | 3504 | C | SER L | 63 | 60.387 | 49.146 | -1.139 | 1.00 49.52 | L | C |
| | MOTA | 3505 | 0 | SER L | 63 | 60.260 | 50.204 | -0.588 | 1.00 50.14 | L | |
| | MOTA | 3506 | \mathbf{N} | GLY L | 64 | 60.505 | 48.022 | -0.459 | 1.00 49.55 | L | |
| 60 | MOTA | 3507 | CA | GLY L | 64 | 60.236 | 47.981 | 0.966 | 1.00 49.92 | L | |
| | ATOM | 3508 | C | GLY L | 64 | 61.159 | 46.980 | 1.657 | 1.00 50.31 | L | |
| | ATOM | 3509 | 0 | GLY L | 64 | 61.708 | 46.063 | 1.050 | 1.00 51.49 | L | |
| | ATOM | 3510 | N | SER L | 65 | 61.365 | 47.192 | 2.967 | 1.00 50.12 | L | |
| GE. | MOTA | 3511 | CA | SER L | 65 65 | 62.186 | 46.237 | 3.707 | 1.00 51.65 | L | |
| 65 | ATOM ATOM | 3512 3513 | CB OG | SER L SER L | 65 65 | 63.669 63.903 | 46.486 47.880 | 3.393 3.197 | 1.00 51.79 1.00 54.65 | L L | |
| | ATOM | 3513 | C | SER L | 65 | 61.942 | 46.325 | 5.240 | 1.00 54.65 | L L | |
| | ATOM | 3515 | 0 | SER L | 65 | 61.163 | 47.105 | 5.722 | 1.00 52.23 | L L | |
| | ATOM | 3516 | N | GLY L | 66 | 62.640 | 45.355 | 5.896 | 1.00 53.83 | L | |
| | | | | | - • | -2.520 | | | | | |

| | | | | | | | | | - | |
|-----|--------------|------------------|------------------------|-------------|------------------|------------------|------------------|--------------------------|--------------|--------|
| | MOTA | | A GLY L | 66 | 62.944 | 45.167 44.044 | 7.285 7.895 | 1.00 54.65 1.00 55.40 | L L | C C |
| | ATOM | 3518 C 3519 O | | 66 66 | 62.097 61.401 | 43.294 | 7.225 | 1.00 56.17 | L | 0 |
| | ATOM ATOM | 3520 N | | 67 | 62.236 | 43.937 | 9.219 9.898 | 1.00 56.74 1.00 57.00 | L L | C N |
| 5 | MOTA | | A SER L | 67 | 61.469 62.289 | 42.901 41.610 | 9.899 | 1.00 56.12 | Ē | C |
| | MOTA MOTA | | CB SER L OG SER L | 67 67 | 63.440 | 41.777 | 10.728 | 1.00 52.42 | Ŀ | 0 |
| | MOTA | 3524 C | | 67 | 61.112 | 43.301 | 11.330 | 1.00 58.80 1.00 58.14 | L L | C C |
| | MOTA | 3525 C | | 67 68 | 61.566 60.226 | 44.299 42.492 | 11.869 11.938 | 1.00 50.14 | L | N |
| 10 | ATOM ATOM | 3526 N 3527 C | N ARG L CA ARG L | 68 | 59.752 | 42.799 | 13.284 | 1.00 62.85 | L | C C |
| | MOTA | | CB ARG L | 68 | 60.943 | 42.830 | 14.243 15.635 | 1.00 66.36 1.00 71.20 | L L | G |
| | MOTA | | CG ARG L | 68 68 | 60.579 61.290 | 42.311 40.988 | 15.902 | 1.00 75.53 | L | С |
| 4.5 | ATOM ATOM | | CD ARG L NE ARG L | 68 | 62.250 | 40.757 | 14.819 | 1.00 79.27 | L | N C |
| 15 | ATOM | | CZ ARG L | 68 | 62.796 | 39.537 | 14.706 15.563 | 1.00 81.84 1.00 81.92 | L L | N |
| | ATOM | | NH1 ARG L NH2 ARG L | 68 68 | 62.477 63.640 | 38.584 39.287 | 13.702 | 1.00 82.11 | L | N |
| | MOTA MOTA | | NH2 ARG L C ARG L | 68 | 59.054 | 44.151 | 13.354 | 1.00 62.53 | L | C O |
| 20 | ATOM | | O ARG L | 68 | 58.092 | 44.438 44.980 | 12.659 14.275 | 1.00 63.47 1.00 61.15 | L L | И |
| | MOTA | | N THR L CA THR L | 69 69 | 59.568 58.935 | 46.256 | 14.555 | 1.00 58.99 | \mathbf{L} | C |
| | MOTA MOTA | | CA THR L CB THR L | 69 | 59.128 | 46.541 | 16.044 | 1.00 60.19 | L L | C O |
| | ATOM | 3540 | OG1 THR L | 69 | 60.474 | 46.226 45.666 | 16.405 16.872 | 1.00 62.69 1.00 59.57 | L | č |
| 25 | MOTA | | CG2 THR L | 69 69 | 58.185 59.549 | 47.398 | 13.734 | 1.00 56.96 | L | C |
| | MOTA MOTA | | O THR L | 69 | 59.270 | 48.573 | 13.949 | 1.00 58.32 1.00 54.09 | L L | O N |
| | MOTA | 3544 | N ASP L | 70 | 60.444 61.095 | 47.031 48.083 | 12.793 12.018 | 1.00 54.09 1.00 52.20 | L | Č |
| 00 | MOTA | | CA ASP L CB ASP L | 70 70 | 62.565 | 48.163 | 12.433 | 1.00 55.60 | L | C |
| 30 | MOTA MOTA | | CG ASP L | 70 | 62.648 | 48.807 | 13.817 | 1.00 58.39 1.00 59.55 | L L | C |
| | MOTA | | OD1 ASP L | 70 | 62.032 63.304 | 49.860 48.254 | 13.992 14.694 | 1.00 59.35 | ŗ | 0 |
| | MOTA ATOM | | OD2 ASP L C ASP L | 70 70 | 60.963 | 47.857 | 10.511 | 1.00 50.32 | L | C |
| 35 | ATOM | 3551 | O ASP L | 70 | 61.438 | 46.878 | 9.956 9.855 | 1.00 50.21 1.00 47.22 | L L | N O |
| | MOTA | 3552 | N PHE L | 71 71 | 60.236 60.062 | 48.803 48.762 | 8.391 | 1.00 45.44 | r L | C |
| | MOTA MOTA | 3553 3554 | CA PHE L | 71 | 58.633 | 48.313 | 8.064 | 1.00 43.23 | L | C |
| | MOTA | 3555 | CG PHE L | 71 | 58.375 | 46.958 | 8.652 9.913 | 1.00 43.34 1.00 41.62 | L L | C |
| 40 | MOTA | 3556 | CD1 PHE L CD2 PHE L | 71 71 | 57.803 58.728 | 46.861 45.818 | 7.952 | 1.00 42.49 | L | C |
| | MOTA MOTA | 3557 3558 | CD2 PHE L CE1 PHE L | 71 | 57.594 | 45.613 | 10.480 | 1.00 40.34 | L L | C |
| | ATOM | 3559 | CE2 PHE L | 71 | 58.515 | 44.567 44.461 | 8.526 9.794 | 1.00 41.49 1.00 41.13 | P P | Č |
| | MOTA | 3560 3561 | CZ PHE L | | 57.955 60.331 | 50.125 | 7.733 | 1.00 45.21 | \mathbf{L} | C |
| 45 | MOTA MOTA | 3561 3562 | O PHE L | | 60.172 | 51.183 | 8.328 | 1.00 46.58 | r r | N O |
| | MOTA | 3563 | N THR L | | 60.799 60.899 | 50.060 51.279 | 6.469 5.668 | 1.00 44.20 1.00 45.03 | L | Ĉ |
| | MOTA | 3564 3565 | CA THR L | | 62.369 | 51.709 | 5.571 | 1.00 46.32 | L | C |
| 50 | ATOM ATOM | 3566 | OG1 THR L | 72 | 63.003 | 51.009 | 4.500 | | L L | O C |
| | MOTA | 3567 | CG2 THR L | 72 | 63.107 60.311 | | 6.874 4.266 | | L | č |
| | ATOM ATOM | 3568 3569 | C THR L | | 60.368 | | 3.684 | 1.00 43.76 | Ŀ | 0 |
| | MOTA | 3570 | N LEU I | . 73 | 59.865 | 52.169 | 3.622 2.296 | | L L | N C |
| 55 | MOTA | 3571 | CA LEU I | | 59.338 57.998 | | 2.268 | | L | C |
| | MOTA MOTA | 3572 3573 | CB LEU I | | 57.448 | | 0.879 | 1.00 40.67 | L | C |
| | ATOM | 3574 | CD1 LEU I | <u>.</u> 73 | 57.165 | | | | L L | C |
| | MOTA | 3575 | CD2 LEU I | | 56.164 60.244 | | | | L | С |
| 60 | MOTA MOTA | 3576 3577 | C LEU I | | 60.489 | | 2.145 | 1.00 40.33 | Ŀ | O |
| | ATOM | 3578 | N THR I | L 74 | 60.745 | | | | L L | N C |
| | MOTA | 3579 | CA THR I | | 61.678 63.014 | | | 3 1.00 45.29 | L | С |
| e E | MOTA MOTA | 3580 3581 | CB THR DOG THR D | | 63.448 | 52.846 | 0.943 | 3 1.00 47.02 | L | 0 |
| 65 | MOTA | 3582 | CG2 THR | ւ 74 | 64.004 | 1 53.738 | | | L L | C |
| | MOTA | | C THR | | 61.192 60.57 | | | 1.00 48.07 | L | 0 |
| | ATOM ATOM | | O THR : | | 61.23 | | | | L | N |
| | AIOM | 3303 | _, | | 220 | | | | | |

| | MOTA | 3586 | CA ILE L | 75 | 60.824 | 55.801 -3.394 | 1.00 49.37 1.00 49.66 | ŗ | C |
|-------|--------------|--------------|------------------------|----------|------------------|----------------------------------|--------------------------|----------|---------|
| | MOTA | 3587 | CB ILE L | 75 75 | 59.716 | 56.813 -3.255 57.029 -4.756 | 1.00 49.00 | L L | C |
| | MOTA | 3588 | CG2 ILE L CG1 ILE L | 75 75 | 59.075 | 56.280 -2.371 | 1.00 48.29 | L L | C |
| E | MOTA | 3589 3590 | CG1 ILE L CD1 ILE L | 75 75 | 58.597 57.615 | 57.253 -2.112 | 1.00 49.44 | L | C |
| 5 | MOTA | 3591 | C ILE L | 75 75 | 62.057 | 56.414 -4.104 | 1.00 51.18 | L L | Č |
| | ATOM ATOM | 3591 | O ILE L | 75 75 | 62.647 | 57.343 -3.656 | 1.00 49.95 | Ŀ | Ö |
| | ATOM | 3593 | N ASN L | 76 | 62.551 | 55.697 -5.093 | 1.00 54.36 | L | Ŋ |
| | ATOM | 3594 | CA ASN L | 76 | 63.754 | 56.088 -5.754 | 1.00 56.06 | L | Ċ |
| 10 | ATOM | 3595 | CB ASN L | 76 | 64.910 | 55.467 -5.119 | 1.00 56.78 | L L | Č |
| 10 | ATOM | 3596 | CG ASN L | 76 | 66.156 | 56.228 -5.432 | 1.00 58.44 | L | Ċ |
| | ATOM | 3597 | OD1 ASN L | 76 | 66.083 | 57.367 -5.916 | 1.00 61.35 | L | 0 |
| | ATOM | 3598 | ND2 ASN L | 76 | 67.262 | 55.617 -5.265 | 1.00 57.10 | L | N |
| | ATOM | 3599 | C ASN L | 76 | 63.854 | 55.739 -7.120 | 1.00 56.03 | L | C |
| 15 | ATOM | 3600 | O ASN L | 76 | 63.964 | 54.552 -7.421 | 1.00 57.71 | L | 0 |
| | MOTA | 3601 | N PRO L | 77 | 63.827 | 56.689 -7.994 | 1.00 55.48 | L | N |
| | MOTA | 3602 | CD PRO L | 77 | 64.022 | 56.425 -9.423 | 1.00 54.95 | L | С |
| | MOTA | 3603 | CA PRO L | 77 | 63.654 | 58.118 -7.725 | 1.00 55.35 | L | C |
| | MOTA | 3604 | CB PRO L | 77 | 64.191 | 58.743 -9.015 | 1.00 54.21 | L | C |
| 20 | MOTA | 3605 | CG PRO L | 77 | 63.679 | 57.741 -10.056 | 1.00 54.17 | L | C |
| | MOTA | 3606 | C PRO L | 77 | 62.202 | 58.627 -7.678 | 1.00 55.61 | L | C |
| | ATOM | 3607 | O PRO L | 77 | 61.249 | 58.102 -8.307 | 1.00 55.40 | L | 0 |
| | ATOM | 3608 | N VAL L | 78 | 62.090 | 59.733 -6.904 | 1.00 55.66 | L | N |
| | MOTA | 3609 | CA VAL L | 78 70 | 60.826 | 60.404 -6.770 | 1.00 55.06 | L L | C |
| 25 | ATOM | 3610 | CB VAL L | 78 78 | 60.878 59.649 | 61.341 -5.622 62.191 -5.632 | 1.00 55.08 1.00 54.52 | L | C |
| | MOTA | 3611 | CG1 VAL L CG2 VAL L | 78 78 | 60.814 | 60.506 -4.300 | 1.00 54.52 | L | C |
| | MOTA | 3612 3613 | | 78 | 60.384 | 61.046 -8.097 | 1.00 54.90 | Ŀ | č |
| | ATOM | 3614 | C VAL L | 78 | 61.125 | 61.666 -8.805 | 1.00 55.13 | L | ŏ |
| 30 | ATOM ATOM | 3615 | N GLU L | 79 | 59.115 | 61.027 -8.313 | 1.00 53.45 | L | N |
| 30 | ATOM | 3616 | CA GLU L | 79 | 58.568 | 61.857 -9.363 | 1.00 53.76 | L | Ĉ |
| | ATOM | 3617 | CB GLU L | 79 | 58.064 | 60.856 -10.490 | 1.00 55.61 | L | Ċ |
| | ATOM | 3618 | CG GLU L | 79 | 59.101 | 59.872 -10.986 | 1.00 59.25 | Ŀ | С |
| | ATOM | 3619 | CD GLU L | 79 | 58.606 | 58.946 -12.112 | 1.00 61.38 | L | C |
| 35 | ATOM | 3620 | OE1 GLU L | 79 | 59.547 | 58.243 -12.667 | 1.00 62.40 | L | 0 |
| | MOTA | 3621 | OE2 GLU L | 79 | 57.390 | 59.009 -12.468 | 1.00 61.93 | L | 0 |
| | ATOM | 3622 | C GLU L | 79 | 57.313 | 62.583 -8.913 | 1.00 52.66 | L | С |
| | MOTA | 3623 | O GLU L | 79 | 56.708 | 62.213 -7.941 | 1.00 52.31 | Ŀ | 0 |
| | MOTA | 3624 | N ALA L | 80 | 56.865 | 63.435 -9.740 | 1.00 52.07 | L | N |
| 40 | MOTA | 3625 | CA ALA L | 80 | 55.877 | 64.405 -9.435 | 1.00 52.18 | <u>L</u> | C |
| | MOTA | 3626 | CB ALA L | 80 | 55.736 | 65.167 -10.630 | 1.00 52.09 | Ŀ | C |
| | MOTA | 3627 | C ALA L | 80 | 54.499 | 63.900 -9.041 | 1.00 51.76 | L | C |
| | MOTA | 3628 | O ALA L | 80 | 53.863 | 64.489 -8.186 | 1.00 49.52 | L | O NT |
| 4 100 | MOTA | 3629 | N ASP L | 81 | 54.106 | 62.824 -9.738 62.079 -9.383 | 1.00 51.07 1.00 52.00 | L L | N C |
| 45 | MOTA | 3630 | CA ASP L | 81 | 52.991 | | 1.00 54.54 | L L | C |
| | ATOM | 3631 | CB ASP L | 81 | 52.635 51.245 | 61.150 -10.581 60.565 -10.455 | 1.00 54.34 | L | C |
| | ATOM | 3632 3633 | CG ASP L | 81 81 | 50.181 | 61.322 -10.285 | 1.00 58.70 | L | ŏ |
| | ATOM ATOM | 3634 | OD1 ASP L OD2 ASP L | 81 | 51.146 | 59.343 -10.407 | 1.00 59.75 | L | ŏ |
| 50 | ATOM | 3635 | C ASP L | 81 | 53.025 | 61.238 -8.054 | 1.00 50.63 | L | č |
| 50 | MOTA | 3636 | O ASP L | 81 | 52.030 | 60.675 -7.720 | 1.00 49.73 | _ L | ō |
| | MOTA | 3637 | N ASP L | 82 | 54.075 | 61.308 -7.279 | 1.00 48.83 | L | N |
| | ATOM | 3638 | CA ASP L | 82 | 54.144 | 60.597 -6.012 | 1.00 48.89 | L | C |
| | MOTA | 3639 | CB ASP L | 82 | 55.588 | 60.276 -5.666 | 1.00 49.88 | L | С |
| 55 | MOTA | 3640 | CG ASP L | 82 | 56.240 | 59.342 -6.753 | 1.00 52.14 | L | C |
| | MOTA | 3641 | OD1 ASP L | 82 | 55.485 | 58.500 -7.287 | 1.00 52.41 | Ŀ | 0 |
| | ATOM | 3642 | OD2 ASP L | 82 | 57.442 | 59.343 -6.965 | 1.00 54.56 | L | 0 |
| | ATOM | 3643 | C ASP L | 82 | 53.673 | 61.396 -4.814 | 1.00 48.65 | ${f L}$ | С |
| | MOTA | 3644 | O ASP L | 82 | 53.819 | 60.947 -3.655 | 1.00 48.04 | L | 0 |
| 60 | MOTA | 3645 | N VAL L | 83 | 53.079 | 62.560 -5.096 | 1.00 47.12 | Ŀ | N |
| | MOTA | 3646 | CA VAL L | 83 | 52.638 | 63.357 -4.005 | 1.00 46.76 | Ē | C |
| | MOTA | 3647 | CB VAL L | 83 | 52.165 | 64.848 -4.323 | 1.00 47.54 | Ŀ | C |
| | MOTA | 3648 | CG1 VAL L | 83 | 53.180 | 65.486 -5.076 | 1.00 48.00 | Ŀ | C |
| | MOTA | 3649 | CG2 VAL L | 83 | 51.050 | 64.877 -5.086 | 1.00 48.87 | ŗ | C |
| 65 | ATOM | 3650 | C VAL L | 83 | 51.408 | 62.654 -3.519 | 1.00 45.32 | L | C |
| | ATOM | 3651 | O VAL L | 83 | 50.459 | 62.419 -4.303 | 1.00 45.55 1.00 43.63 | · L | O |
| | MOTA | 3652 | N ALA L | 84 | 51.466 | 62.377 -2.239 | 1.00 43.63 | L L | N |
| | MOTA | 3653 | CA ALA L | 84 84 | 50.503 50.563 | 61.592 -1.600 60.211 -2.223 | 1.00 42.80 | L L | C |
| | MOTA | 3654 | CB ALA L | 04 | 20.503 | 00.211 -2.223 | T.00 | | _ |

| | ATOM | 3655 | С | 7 T 7 T | 84 | 50.774 | 61.441 | -0.101 | 1.00 41.61 | т | ~ |
|----|--------------|--------------|----------|----------------|----------|------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM | 3656 | 0 | ALA L ALA L | 84 | 51.894 | 61.441 | 0.329 | 1.00 42.11 | L L | C |
| | ATOM | 3657 | N | THR L | 85 | 49.863 | 60.727 | 0.565 | 1.00 39.60 | L | И |
| | ATOM | 3658 | ĈA | THR L | 85 | 50.123 | 60.302 | 1.982 | 1.00 41.07 | L | C |
| 5 | ATOM | 3659 | CB | THR L | 85 | 48.924 | 60.597 | 2.859 | 1.00 41.88 | L | Č |
| | MOTA | 3660 | OG1 | THR L | 85 | 48.909 | 61.984 | 2.953 | 1.00 43.50 | L | 0 |
| | MOTA | 3661 | CG2 | THR L | 85 | 49.099 | 60.169 | 4.220 | 1.00 42.73 | L | C |
| | MOTA | 3662 | С | THR L | 85 | 50.389 | 58.812 | 1.925 | 1.00 41.86 | L | C |
| | ATOM | 3663 | 0 | THR L | 85 | 49.688 | 58.201 | 1.232 | 1.00 42.14 | L | 0 |
| 10 | ATOM | 3664 | N | TYR L | 86 | 51.335 | 58.228 | 2.692 | 1.00 41.17 | L | N |
| | MOTA | 3665 | CA | TYR L | 86 86 | 51.669 | 56.827 56.644 | 2.666 | 1.00 42.15 | L | C |
| | ATOM ATOM | 3666 3667 | CB CG | TYR L | 86 86 | 53.123 53.481 | 57.131 | $2.243 \\ 0.849$ | 1.00 40.67 1.00 40.33 | L L | C |
| | ATOM | 3668 | | | 86 | 53.696 | 58.456 | 0.549 | 1.00 40.33 | L | C |
| 15 | MOTA | 3669 | CE1 | TYR L | 86 | 53.913 | 58.828 | -0.781 | 1.00 38.35 | L | Ċ |
| | ATOM | 3670 | CD2 | TYR L | 86 | 53.330 | 56.289 | -0.211 | 1.00 38.76 | L | Č |
| | ATOM | 3671 | CE2 | TYR L | 86 | 53.525 | 56.769 | -1.598 | 1.00 37.31 | L | C |
| | MOTA | 3672 | CZ | TYR L | 86 | 53.794 | 58.033 | -1.809 | 1.00 40.02 | L | С |
| 4 | ATOM | 3673 | OH | TYR L | 86 | 53.888 | 58.480 | -3.251 | 1.00 37.67 | L | 0 |
| 20 | ATOM | 3674 | C | TYR L | 86 | 51.398 | 56.221 | 3.934 | 1.00 44.14 | L | C |
| | MOTA | 3675 | O | TYR L | 86 | 51.819 | 56.826 | 5.017 | 1.00 46.29 | Ļ | 0 |
| | ATOM ATOM | 3676 3677 | N CA | TYR L | 87 87 | 50.679 50.454 | 55.064 54.392 | 3.945 5.249 | 1.00 42.51 1.00 42.40 | L L | C N |
| | ATOM | 3678 | CB | TYR L | 87 | 48.946 | 54.323 | 5.530 | 1.00 42.40 | L | C |
| 25 | ATOM | 3679 | CG | TYR L | 87 | 48.195 | 55.573 | 5.499 | 1.00 39.25 | L | Č |
| | MOTA | 3680 | CD1 | TYR L | 87 | 47.708 | 56.110 | 4.322 | 1.00 37.90 | L | Ċ |
| | ATOM | 3681 | CE1 | TYR L | 87 | 46.929 | 57.277 | 4.400 | 1.00 37.86 | L | С |
| | MOTA | 3682 | CD2 | TYR L | 87 | 47.710 | 56.086 | 6.696 | 1.00 39.45 | L | C |
| | MOTA | 3683 | CE2 | TYR L | 87 | 47.057 | 57.273 | 6.743 | 1.00 37.41 | L | C |
| 30 | ATOM | 3684 | CZ | TYR L | 87 | 46.626 | 57.829 | 5.430 | 1.00 37.62 | Ţ. | C |
| | ATOM ATOM | 3685 3686 | OH C | TYR L TYR L | 87 87 | 45.851 50.917 | 58.916 52.985 | 5.440 5.331 | 1.00 40.72 1.00 43.25 | L L | О С |
| | ATOM | 3687 | 0 | TYR L | 87 | 50.917 | 52.298 | 4.273 | 1.00 43.23 | L | .0 |
| | MOTA | 3688 | N | CYS L | 88 | 51.324 | 52.585 | 6.557 | 1.00 44.13 | L | N |
| 35 | ATOM | 3689 | CA | CYS L | 88 | 51.632 | 51.249 | 6.833 | 1.00 44.88 | L | Ĉ |
| | ATOM | 3690 | C | CYS L | 88 | 50.505 | 50.617 | 7.597 | 1.00 44.55 | L | C |
| | ATOM | 3691 | 0 | CYS L | 88 | 49.622 | 51.295 | 8.129 | 1.00 43.38 | L | 0 |
| | ATOM | 3692 | CB | CYS L | 88 | 52.986 | 51.039 | 7.654 | 1.00 44.75 | L | C |
| 40 | ATOM | 3693 | SG | CYS L | 88 | 52.928 | 52.042 | 9.185 | 1.00 45.57 | Ŀ | S |
| 40 | ATOM | 3694 | N | GLN L | 89 | 50.460 | 49.282 | 7.528 | 1.00 44.18 | L | N |
| | ATOM ATOM | 3695 3696 | CA CB | GLN L GLN L | 89 89 | 49.292 48.125 | 48.540 48.523 | 8.105 7.140 | 1.00 44.10 1.00 42.71 | L L | C |
| | ATOM | 3697 | CG | GLN L | 89 | 46.971 | 47.793 | 7.704 | 1.00 42.71 | L | C |
| | ATOM | 3698 | CD | GLN L | 89 | 46.825 | 46.370 | 6.956 | 1.00 42.95 | L | č |
| 45 | ATOM | 3699 | OE1 | GLN L | 89 | 46.839 | 46.258 | 5.730 | 1.00 41.37 | L | ō |
| | ATOM | 3700 | NE2 | GLN L | 89 | 46.888 | 45.307 | 7.793 | 1.00 38.44 | L | N |
| | ATOM | 3701 | С | GLN L | 89 | 49.756 | 47.136 | 8.424 | 1.00 45.06 | L | С |
| | ATOM | 3702 | 0 | GLN L | 89 | 50.446 | 46.580 | 7.598 | 1.00 44.95 | L | 0 |
| 50 | ATOM | 3703 | N | GLN L | 90 | 49.475 | 46.672 | 9.633 | 1.00 44.17 | L | N |
| 50 | ATOM ATOM | 3704 3705 | CA CB | GLN L GLN L | 90 90 | 49.737 50.491 | 45.307 45.296 | 10.051 11.398 | 1.00 44.79 1.00 42.34 | L L | C |
| | ATOM | 3705 | CG | GLN L | 90 | 49.625 | 45.801 | 12.585 | 1.00 44.52 | T T | C |
| | MOTA | 3707 | CD | GLN L | 90 | 48.654 | 44.710 | 13.155 | 1.00 46.51 | L | Č |
| | MOTA | 3708 | OE1 | GLN L | 90 | 48.921 | 43.583 | 13.018 | 1.00 46.93 | L | Ō |
| 55 | ATOM | 3709 | NE2 | GLN L | 90 | 47.546 | 45.105 | 13.756 | 1.00 46.47 | L | N |
| | MOTA | 3710 | C | GLN L | 90 | 48.505 | 44.352 | 10.090 | 1.00 45.80 | L | С |
| | MOTA | 3711 | 0 | GLN L | 90 | 47.331 | 44.706 | 10.396 | 1.00 44.66 | L | 0 |
| | MOTA | 3712 | N | SER L | 91 | 48.793 | 43.072 | 9.763 | 1.00 47.04 | Ţ | N |
| 60 | MOTA | 3713 | CA | SER L | 91 | 47.841 | 42.007 | 9.605 | 1.00 50.24 1.00 50.88 | L | C |
| 60 | ATOM ATOM | 3714 3715 | CB OG | SER L SER L | 91 91 | 47.991 47.148 | 41.516 42.515 | $8.052 \\ 7.448$ | 1.00 50.88 | L L | C |
| | ATOM | 3716 | C | SER L | 91 | 48.260 | 40.852 | 10.535 | 1.00 51.02 | Г | Č |
| | ATOM | 3717 | ŏ | SER L | 91 | 47.818 | 39.741 | 10.359 | 1.00 51.43 | L | ŏ |
| | ATOM | 3718 | N | ASN L | 92 | 49.096 | 41.136 | 11.526 | 1.00 51.69 | Ľ | N |
| 65 | MOTA | 3719 | CA | ASN L | 92 | 49.553 | 40.106 | 12.404 | 1.00 52.68 | L | C |
| | MOTA | 3720 | CB | ASN L | 92 | 50.955 | 40.293 | 12.867 | 1.00 53.64 | L | С |
| | ATOM | 3721 | CG | ASN L | 92 | 51.439 | 39.102 | 13.659 | 1.00 54.66 | L | C |
| | MOTA | 3722 | | ASN L | 92 | 51.345 | 38.022 | 13.199 | 1.00 55.46 | L | O |
| | ATOM | 3723 | אחא | ASN L | 92 | 52.089 | 39.337 | 14.773 | 1.00 53.66 | Ŀ | N |

| | ATOM | 3724 | C ASN L | 92 | 48.650 | 39.774 | 13.452 | 1.00 52.84 | Ţ | C |
|----|--------------|--------------|------------------------|----------|------------------|------------------|------------------|--------------------------|--------------|--------|
| | MOTA | 3725 | O ASN L | 92 | 48.547 | 38.677 | 13.787 | 1.00 51.48 1.00 54.21 | L L | O N |
| • | MOTA | 3726 | N GLU L | 93 93 | 47.867 46.917 | 40.694 40.511 | 13.784 14.847 | 1.00 56.33 | L | C |
| 5 | ATOM ATOM | 3727 3728 | CA GLU L CB GLU L | 93 | 47.664 | 40.794 | 16.127 | 1.00 58.27 | L | Č |
| 5 | MOTA | 3729 | CG GLU L | 93 | 46.781 | 41.352 | 17.225 | 1.00 64.91 | L | C |
| | MOTA | 3730 | CD GLU L | 93 | 47.570 | 41.631 | 18.613 | 1.00 69.27 | L | С |
| | MOTA | 3731 | OE1 GLU L | 93 | 47.033 | 42.328 | 19.596 | 1.00 69.83 | Ŀ | 0 |
| | MOTA | 3732 | OE2 GLU L | 93 | 48.753 | 41.164 | 18.679 | 1.00 71.16 1.00 55.46 | L L | 0 |
| 10 | ATOM | 3733 | C GLU L | 93 | 45.693 45.830 | 41.403 42.487 | 14.792 14.512 | 1.00 55.46 1.00 55.13 | L | Ö |
| | MOTA ATOM | 3734 3735 | O GLU L N ASP L | 93 94 | 44.532 | 40.975 | 15.329 | 1.00 54.53 | L | Ň |
| | ATOM | 3736 | CA ASP L | 94 | 43.346 | 41.750 | 15.364 | 1.00 53.23 | L | C |
| • | ATOM | 3737 | CB ASP L | 94 | 42.142 | 40.809 | 15.294 | 1.00 54.70 | L | С |
| 15 | MOTA | 3738 | CG ASP L | 94 ' | 42.076 | 39.997 | 13.826 | 1.00 57.43 | L | C |
| | MOTA | 3739 | OD1 ASP L | 94 | 42.696 | 40.310 | 12.814 | 1.00 57.14 1.00 61.04 | L L | 0 |
| | MOTA | 3740 | OD2 ASP L | 94 | 41.463 43.190 | 39.008 42.589 | 13.648 16.555 | 1.00 51.04 | P. | Č |
| | MOTA | 3741 3742 | C ASP LOOK | 94 94 | 43.190 | 42.180 | 17.663 | 1.00 54.05 | L | ŏ |
| 20 | ATOM ATOM | 3742 | N PRO L | 95 | 42.672 | 43.777 | 16.387 | 1.00 48.83 | L | N |
| 20 | ATOM | 3744 | CD PRO L | 95 | 42.461 | 44.714 | 17.489 | 1.00 47.99 | \mathbf{L} | C |
| | ATOM | 3745 | CA PRO L | 95 | 42.312 | 44.348 | 15.087 | 1.00 48.09 | L | C |
| | MOTA | 3746 | CB PRO L | 95 | 41.376 | 45.510 | 15.436 | 1.00 49.09 | L | C |
| | MOTA | 3747 | CG PRO L | 95 | 42.063 | 46.117 | 16.791 | 1.00 47.71 | L L | C |
| 25 | ATOM | 3748 | C PRO L | 95 | 43.396 44.300 | 44.759 45.389 | 14.188 14.643 | 1.00 46.87 1.00 47.73 | L | Ö |
| | ATOM | 3749 3750 | O PRO L N TRP L | 95 96 | 43.354 | 44.392 | 12.867 | 1.00 47.73 | L | N |
| | ATOM ATOM | 3750 3751 | N TRP L CA TRP L | 96 | 44.289 | 45.074 | 11.947 | 1.00 45.52 | L | Ċ |
| | ATOM | 3752 | CB TRP L | 96 | 44.003 | 44.780 | 10.478 | 1.00 45.68 | L | C |
| 30 | ATOM | 3753 | CG TRP L | 96 | 44.181 | 43.372 | 10.097 | 1.00 45.86 | L | C |
| | ATOM | 3754 | CD2 TRP L | 96 | 44.084 | 42.815 | 8.827 | 1.00 46.64 | L | C |
| | ATOM | 3755 | CE2 TRP L | 96 | 44.231 | 41.361 | 8.976 | 1.00 46.98 | L | C |
| | MOTA | 3756 | CE3 TRP L | 96 | 43.831 | 43.331 | 7.577 | 1.00 47.58 1.00 44.89 | L L | C |
| | MOTA | 3757 | CD1 TRP L | 96 | 44.369 44.446 | 42.327 41.119 | 10.941 10.306 | 1.00 45.59 | L | N |
| 35 | MOTA | 3758 3759 | NE1 TRP L CZ2 TRP L | 96 96 | 44.327 | 40.521 | 7.939 | 1.00 46.28 | L | Ĉ |
| | ATOM ATOM | 3760 | CZZ TRP L | 96 | 43.875 | 42.467 | 6.467 | 1.00 48.84 | L | С |
| | ATOM | 3761 | CH2 TRP L | 96 | 44.030 | 41.022 | 6.640 | 1.00 47.17 | L | C |
| | MOTA | 3762 | C TRP L | 96 | 44.304 | 46.639 | 12.165 | 1.00 43.70 | L | C |
| 40 | MOTA | 3763 | O TRP L | 96 | 43.282 | 47.212 | 12.334 | 1.00 42.66 | ŗ | 0 |
| | MOTA | 3764 | N THR L | 97 | 45.480 | 47.279 | 12.172 | 1.00 42.35 1.00 42.63 | L L | N C |
| | ATOM | 3765 | CA THR L | 97 | 45.610 46.179 | 48.692 49.032 | 12.325 13.645 | 1.00 42.03 | L | Ċ |
| | MOTA | 3766 | CB THR L | 97 97 | 47.337 | 48.270 | 13.806 | 1.00 42.43 | L | ŏ |
| 45 | MOTA MOTA | 3767 3768 | CG2 THR L | 97 | 45.190 | 48.602 | 14.784 | 1.00 42.15 | L | C |
| 40 | MOTA | 3769 | C THR L | 97 | 46.561 | 49.331 | 11.315 | 1.00 42.11 | L | С |
| | MOTA | 3770 | O THR L | 97 | 47.465 | 48.653 | 10.852 | 1.00 40.72 | L | 0 |
| | MOTA | 3771 | N PHE L | 98 | 46.371 | 50.620 | 11.204 | 1.00 42.79 | ŗ | |
| | MOTA | 3772 | CA PHE L | 98 | 47.158 | 51.355 | 10.243 | 1.00 44.72 1.00 44.19 | L L | C |
| 50 | ATOM | 3773 | CB PHE L | 98 98 | 46.257 45.492 | 52.157 51.275 | 9.301 8.233 | 1.00 44.19 | Ŀ | C |
| | MOTA MOTA | 3774 3775 | CG PHE L CD1 PHE L | 98 | 44.260 | 50.690 | 8.549 | 1.00 44.38 | L | Č |
| | ATOM | 3776 | CD1 PHE L | 98 | 45.845 | 51.317 | 6.909 | 1.0043.71 | L | С |
| | ATOM | 3777 | CE1 PHE L | 98 | 43.579 | 49.891 | 7.630 | 1.00 44.14 | L | С |
| 55 | ATOM | 3778 | CE2 PHE L | 98 | 45.142 | 50.544 | 5.952 | 1.00 44.40 | L | C |
| | MOTA | 3779 | CZ PHE L | 98 | 43.990 | 49.844 | 6.323 | 1.00 43.77 | Ŀ | C |
| | ATOM | 3780 | C PHE L | 98 | 48.021 | 52.424 | 11.032 | 1.00 45.39 1.00 46.17 | Ŀ L | C 0 |
| | ATOM | 3781 | O PHE L | 98 | 47.539 | 53.020 52.858 | 11.932 10.467 | 1.00 45.17 | Ŀ | |
| 60 | ATOM | 3782 | N GLY L | 99 99 | 49.155 49.809 | 54.075 | 10.407 | 1.00 45.06 | L | Ĉ |
| 60 | ATOM ATOM | 3783 3784 | CA GLY L C GLY L | 99 99 | 49.051 | 55.337 | 10.565 | 1.00 46.31 | Ĺ | |
| | ATOM | 3785 | O GLY L | 99 | 48.143 | 55.392 | 9.509 | 1.00 45.42 | L | 0 |
| | ATOM | 3786 | N GLY L | | 49.531 | 56.441 | 11.247 | 1.00 45.88 | L | |
| | MOTA | 3787 | CA GLY L | | 49.024 | 57.752 | 11.058 | 1.00 45.30 | Ŀ | |
| 65 | ATOM | 3788 | C GLY L | 100 | 49.199 | 58.373 | 9.657 | 1.00 45.43 | L | |
| | MOTA | 3789 | O GLY L | | 48.790 | 59.443 | 9.313 | 1.00 45.57 1.00 45.62 | L L | |
| | ATOM | 3790 | N GLY L | | 50.013 | 57.757 58.406 | 8.844 7.650 | 1.00 45.85 | r T | |
| | MOTA | 3791 | CA GLY L | | 50.426 51.663 | 59.279 | 7.620 | 1.00 45.85 | L | |
| | MOTA | 3792 | C GLY L | TOT | 24.002 | 33.213 | , | | _ | |

| | ATOM | 3793 | 0 | GLY L 101 | | 51.934 | 59.904 | 8.587 | 1.00 44.61 | L | 0 |) |
|-----|--------------|--------------|-----------|------------------------|---------------|------------------|------------------|-------------------|--------------------------|--------|--------|--------|
| | MOTA | 3794 | N | THR L 102 | | 52.291 | 59.442 | 6.433 | 1.00 45.36 | L | N | |
| | MOTA | 3795 | | THR L 102 THR L 102 | | 53.411 54.626 | 60.313 59.534 | 6.255 5.965 | 1.00 45.28 1.00 44.83 | L L | C | |
| 5 | MOTA MOTA | 3796 3797 | CB OG1 | THR L 102 | | 55.236 | 59.086 | 7.115 | 1.00 44.03 | L | 0 |) |
| J | MOTA | 3798 | CG2 | THR L 102 | | 55.665 | 60.329 | 5.172 | 1.00 44.01 1.00 46.66 | L L | C | |
| | ATOM | 3799 | C | THR L 102 THR L 102 | | 53.154 52.867 | 60.976 60.240 | 4.830 3.841 | 1.00 45.35 | L | o | |
| | ATOM ATOM | 3800 3801 | N O | LYS L 103 | | 53.058 | 62.320 | 4.809 | 1.00 47.18 | L | N | |
| 10 | MOTA | 3802 | CA | LYS L 103 | | 52.816 | 63.201 | 3.673 | 1.00 48.50 1.00 50.90 | L L | d | |
| | MOTA | 3803 3804 | CB CG | LYS L 103 LYS L 103 | | 52.191 51.609 | 64.445 65.477 | $4.212 \\ 3.221$ | 1.00 56.57 | L | d | |
| | ATOM ATOM | 3804 | CD | LYS L 103 | | 50.967 | 64.749 | 1.911 | 1.00 60.51 | L | C | 3 |
| | ATOM | 3806 | CE | LYS L 103 | | 50.587 | 65.501 | 0.527 | 1.00 60.75 | L L | N. | |
| 15 | MOTA | 3807 | NZ | LYS L 103 | | 49.218 54.089 | 64.661 63.528 | 0.158 2.937 | 1.00 64.51 1.00 49.12 | r L | | |
| | MOTA MOTA | 3808 3809 | C O | LYS L 103 | | 55.070 | 63.987 | 3.529 | 1.00 46.89 | L | C |) |
| | ATOM | 3810 | N | LEU L 104 | | 54.136 | 63.203 | 1.640 | 1.00 49.88 1.00 50.17 | L L | | |
| | MOTA | 3811 | CA | LEU L 104 LEU L 104 | | 55.237 55.450 | 63.493 62.279 | 0.821 -0.094 | 1.00 50.17 | L | | |
| 20 | ATOM ATOM | 3812 3813 | CB CG | LEU L 104 | | 56.504 | 62.487 | -1.172 | 1.00 51.61 | L | C | 3 |
| | ATOM | 3814 | CD1 | LEU L 104 | | 57.736 | 62.665 | -0.408 | 1.00 50.91 | L L | | 7 |
| | MOTA | 3815 | | LEU L 104 LEU L 104 | | 56.680 54.886 | 61.293 64.669 | -2.010 -0.160 | 1.00 51.28 1.00 50.51 | L | | ž |
| 25 | MOTA MOTA | 3816 3817 | C O | LEU L 104 | | 54.013 | 64.595 | -0.991 | 1.00 50.36 | L | | С |
| 20 | MOTA | 3818 | N | GLU L 105 | | 55.750 | 65.621 | -0.180 | 1.00 52.49 | L | | N C |
| | MOTA | 3819 | CA | GLU L 105 | | 55.759 55.539 | 66.681 67.921 | -1.104 -0.352 | 1.00 54.11 1.00 55.10 | L L | . (| C |
| | ATOM ATOM | 3820 3821 | CB CG | GLU L 105 GLU L 105 | | 54.018 | 67.996 | -0.086 | 1.00 61.17 | I | , (| С |
| 30 | MOTA | 3822 | CD | GLU L 105 | | 53.637 | 68.790 | 1.207 | 1.00 64.63 | I I | | C O |
| | ATOM | 3823 | OE1 | | | 54.425 52.652 | 68.420 69.661 | 2.179 1.163 | 1.00 67.64 1.00 65.16 | I | | Ö |
| | ATOM ATOM | 3824 3825 | OE2 C | GLU L 105 GLU L 105 | | 56.954 | 66.708 | -2.082 | 1.00 54.00 | I | ı (| С |
| | ATOM | 3826 | ŏ | GLU L 105 | | 58.116 | 66.333 | -1.762 | 1.00 53.00 | I | | O N |
| 35 | ATOM | 3827 | N | ILE L 106 | | 56.644 57.745 | 67.285 67.670 | -3.223 -4.139 | 1.00 54.75 1.00 56.70 | I | | C |
| | MOTA MOTA | 3828 3829 | CA CB | ILE L 106 | | 57.349 | 67.406 | -5.589 | 1.00 56.28 | I | , (| С |
| | ATOM | 3830 | CG2 | ILE L 106 | | 58.592 | 67.703 | -6.534 | 1.00 56.73 | I | | C C |
| | MOTA | 3831 | CG1 | | | 56.777 57.702 | 65.999 65.016 | -5.661 -5.232 | 1.00 57.37 1.00 56.71 | Ī | | C |
| 40 | MOTA MOTA | 3832 3833 | CD1 C | ILE L 106 | | 58.348 | 69.019 | -3.972 | 1.00 57.21 | I | . (| С |
| | ATOM | 3834 | ō | ILE L 106 | | 57.604 | 69.928 | -3.826 | 1.00 57.93 1.00 57.73 | I | | O N |
| | ATOM | 3835 | N | LYS L 107 | | 59.714 60.478 | 69.124 70.430 | -3.982 -4.003 | 1.00 57.73 | I | | C |
| 45 | ATOM ATOM | 3836 3837 | CA CB | LYS L 107 | | 61.787 | 70.552 | -3.283 | 1.00 58.92 | I | | C |
| -10 | ATOM | 3838 | CG | LYS L 107 | | 61.726 | 70.325 | -1.955 | 1.00 61.50 1.00 63.56 | | | C |
| | ATOM | 3839 | CD | LYS L 107 | | 63.145 63.002 | 70.594 71.212 | -1.364 0.071 | 1.00 65.27 | | | C |
| | MOTA MOTA | 3840 3841 | CE NZ | LYS L 107 | , | 64.255 | 71.130 | 0.893 | 1.00 67.17 | | | N |
| 50 | ATOM | 3842 | C | LYS L 107 | ' | 60.785 | 70.780 | -5.419 | 1.00 58.54 1.00 59.83 | | | C |
| | MOTA | 3843 3844 | N O | LYS L 107 ARG L 108 | | 61.079 60.489 | 69.888 72.052 | -6.256 -5.691 | 1.00 57.71 | | | N |
| | MOTA MOTA | 3845 | CA | ARG L 108 | | 60.602 | 72.586 | -6.940 | 1.00 56.79 | | | C |
| | MOTA | 3846 | CB | ARG L 108 | | 59.370 | 72.336 | -7.752 7.303 | 1.00 56.25 1.00 57.11 | | ւ Մ | C |
| 55 | MOTA | 3847 3848 | CG CD | ARG L 108 | } ? | 58.122 57.194 | 72.926 73.347 | -7.302 -8.373 | 1.00 58.22 | | | C |
| | MOTA MOTA | 3849 | NE | ARG L 10 | | 57.728 | 74.544 | -9.051 | 1.00 59.58 | | | N |
| | MOTA | 3850 | CZ | ARG L 10 | | 57.277 | 75.002 | -10.208 | 1.00 60.73 1.00 60.18 | | | N C |
| 00 | MOTA | 3851 | NH: | | 3 | 56.286 57.817 | 74.384 76.093 | -10.896 -10.739 | 1.00 60.18 | | | N |
| 60 | ATOM ATOM | 3852 3853 | NH: C | ARG L 10 | | 61.109 | 73.981 | -6.858 | 1.00 57.20 | : | L | С |
| | MOTA | 3854 | 0 | ARG L 10 | 3 | 61.247 | 74.526 | -5.783 | 1.00 57.37 | | | И О |
| | MOTA | 3855 | | ALA L 10 ALA L 10 | | 61.418 61.799 | | -8.058 -8.199 | 1.00 56.62 1.00 56.09 | | | C |
| 65 | MOTA MOTA | 3856 3857 | | | | 62.040 | | -9.655 | 1.00 53.79 | | L | C |
| | MOTA | 3858 | С | ALA L 10 | 9 | 60.615 | | -7.667 | 1.00 56.43 1.00 56.16 | | | C |
| | MOTA | 3859 | | ALA L 10 ASP L 11 | | 59.410 60.920 | | -7.921 -6.998 | | | | N |
| | MOTA MOTA | 3860 3861 | | | | 59.892 | | | | | L | С |
| | | | | | | 22.4 | | | | | | |

| | | | | | | | 1 00 56 01 | т. | С |
|----|--------------|------------------|--------------------------------|------------------|------------------|----------------------|----------------------------|---------------------|--------|
| | MOTA | 3862 CE | | ο 0.511 | 80.157 79.797 | -5.837 -4.443 | 1.00 56.81 1.00 58.54 | L L | C |
| | MOTA | 3863 CG | ASP L 110 D1 ASP L 110 | 61.128 60.928 | 78.730 | -3.852 | 1.00 59.52 | L | 0 |
| | ATOM ATOM | | 02 ASP L 110 | 61.870 | 80.621 | -3.807 | 1.00 59.92 | L L | 0 |
| 5 | MOTA | 3866 C | ASP L 110 | 59.125 | 79.430 | -7.775 -8.905 | 1.00 57.69 1.00 59.35 | L | 0 |
| | MOTA | 3867 0 | ASP L 110 | 59.672 57.838 | 79.417 79.723 | -7.595 | 1.00 56.11 | L | N |
| | MOTA | 3868 N 3869 C | ALA L 111 A ALA L 111 | 56.869 | 80.171 | -8.619 | 1.00 55.19 | L | C |
| | ATOM ATOM | 3870 CI | | 56.070 | 79.034 | -9.159 | 1.00 52.10 | L L | C |
| 10 | ATOM | 3871 C | ALA L 111 | 55.941 | 81.179 | -7.991 -6.956 | 1.00 55.80 1.00 55.37 | r L | Ö |
| | MOTA | 3872 0 | ALA L 111 | 55.376 55.807 | 80.892 82.368 | -8.618 | 1.00 56.05 | L | N |
| | ATOM | 3873 N 3874 C | | 54.850 | 83.310 | -8.173 | 1.00 56.07 | L | C |
| | MOTA MOTA | 3875 C | | 55.222 | 84.806 | -8.826 | 1.00 55.31 | L L | C |
| 15 | ATOM | 3876 C | ALA L 112 | 53.370 | 82.893 | -8.402 -9.455 | 1.00 56.07 1.00 56.89 | Ŀ | Ö |
| | MOTA | 3877 0 | ALA L 112 | 52.988 52.474 | 82.406 83.234 | -7.505 | 1.00 55.80 | L | N |
| | MOTA | 3878 N 3879 C | PRO L 113 D PRO L 113 | 52.643 | 84.043 | -6.244 | 1.00 54.68 | Ŀ | C |
| | ATOM ATOM | | A PRO L 113 | 51.074 | 83.015 | -7.777 | 1.00 54.69 1.00 54.68 | L L | C |
| 20 | MOTA | | B PRO L 113 | 50.384 | 83.513 | -6.451 -5.848 | 1.00 54.66 | L | Č |
| | MOTA | • | G PRO L 113 PRO L 113 | 51.271 50.516 | 84.529 83.920 | -8.805 | 1.00 54.74 | L | С |
| | MOTA | 3883 C 3884 O | | 50.922 | 85.031 | -8.877 | 1.00 55.39 | $	ilde{\mathbf{r}}$ | O |
| | ATOM ATOM | 3885 N | THR L 114 | 49.392 | 83.530 | -9.334 | 1.00 54.38 1.00 54.72 | L L | N C |
| 25 | MOTA | 3886 C | THR L 114 | 48.631 48.300 | 84.218 83.289 | -10.276 -11.360 | 1.00 54.72 1.00 55.08 | L | č |
| | ATOM | • • • • | CB THR L 114 OG1 THR L 114 | 49.517 | 82.942 | -11.940 | 1.00 56.71 | ${f L}$ | 0 |
| | ATOM ATOM | | OG1 THR L 114 CG2 THR L 114 | 47.352 | 84.010 | -12.458 | 1.00 54.02 | Ŀ | C |
| | MOTA | 3890 C | THR L 114 | 47.315 | 84.529 | -9.570 | 1.00 55.93 1.00 55.95 | L L | Ö |
| 30 | ATOM | 3891 0 | THR L 114 | 46.529 | 83.548 85.831 | -9.242 -9.299 | 1.00 55.11 | Ĺ | N |
| | MOTA | | N VAL L 115 CA VAL L 115 | 47.093 46.026 | 86.296 | -8.435 | 1.00 55.65 | \mathbf{L} | C |
| | MOTA MOTA | • | CA VAL L 115 CB VAL L 115 | 46.526 | 87.339 | -7.568 | 1.00 55.29 | L | C |
| | ATOM | | CG1 VAL L 115 | 45.498 | 87.847 | -6.585 -6.861 | 1.00 54.37 1.00 55.51 | L L | C |
| 35 | MOTA | 3896 (| CG2 VAL L 115 | 47.733 44.896 | 86.748 86.832 | -9.187 | 1.00 56.77 | L | С |
| | MOTA | | C VAL L 115 O VAL L 115 | 45.067 | 87.612 | -10.165 | 1.00 57.49 | L | 0 |
| | MOTA MOTA | | N SER L 116 | 43.697 | 86.493 | -8.747 | 1.00 57.44 | L L | N C |
| | MOTA | | CA SER L 116 | 42.536 | 87.040 | -9.514 -10.433 | 1.00 59.96 1.00 59.44 | P P | C |
| 40 | MOTA | | CB SER L 116 | 41.993 43.127 | 86.004 85.809 | | 1.00 63.37 | L | 0 |
| | MOTA | | OG SER L 116 C SER L 116 | 41.517 | 87.421 | -8.528 | 1.00 61.30 | L | C |
| | MOTA MOTA | • • • • | O SER L 116 | 41.396 | 86.709 | -7.486 | 1.00 62.38 1.00 62.29 | L L | O N |
| | MOTA | 3905 | N ILE L 117 | 40.807 | 88.529 88.949 | | 1.00 62.25 | L | Ĉ |
| 45 | MOTA | | CA ILE L 117 CB ILE L 117 | 39.705 40.034 | | | 1.00 64.24 | L | C |
| | MOTA MOTA | 3907 3908 | CB ILE L 117 CG2 ILE L 117 | 39.911 | 91.545 | -8.193 | 1.00 63.93 | Ŀ | C |
| | MOTA | 3909 | CG1 ILE L 117 | 39.176 | | | 1.00 63.82 1.00 63.17 | L L | C |
| | ATOM | 3910 | CD1 ILE L 117 | 39.509 | | 3 -5.135 7 -8.605 | | L | Č |
| 50 | MOTA | 3911 | C ILE L 117 O ILE L 117 | 38.324 38.135 | | | 1.00 66.10 | L | 0 |
| | MOTA MOTA | 3912 3913 | N PHE L 117 | 37.301 | 88.667 | 7 –7.783 | 1.00 65.70 | L L | N C |
| | ATOM | 3914 | CA PHE L 118 | 36.011 | | | | r L | Č |
| | MOTA | 3915 | CB PHE L 118 | 35.650 36.650 | | | | L | C |
| 55 | MOTA | 3916 | CG PHE L 118 CD1 PHE L 118 | 37.740 | | | 1.00 69.91 | L | C |
| | MOTA MOTA | 3917 3918 | CD2 PHE L 118 | 36.448 | 86.08 | 7 -10.734 | | L | C |
| | ATOM | | CE1 PHE L 118 | 38.640 | | | 1.00 69.94 3 1.00 68.43 | L L | c |
| | MOTA | 3920 | CE2 PHE L 118 | 37.333 38.378 | | | | L | C |
| 60 | ATOM | | CZ PHE L 118 C PHE L 118 | 34.952 | | | 1.00 68.64 | L | C |
| | MOTA | | C PHE L 118 O PHE L 118 | 34.82 | 88.89 | 9 -6.264 | | ŗ | O |
| | MOTA MOTA | | N PRO L 119 | 34.15 | 1 90.10 | 3 -8.063 | | L L | C N |
| | MOTA | 3925 | CD PRO L 119 | 34.18 | | | | Ŀ | C |
| 65 | MOTA | | CA PRO L 119 CB PRO L 119 | 33.09 32.68 | | | 0 1.00 68.71 | L | C |
| | MOTA | | CB PRO L 119 CG PRO L 119 | 33.93 | | 7 -9.08 | 7 1.00 69.40 | L | C |
| | MOTA MOTA | | C PRO L 119 | 31.94 | 1 89.87 | | | L L | C O |
| | ATOM | | O PRO L 119 | 31.81 | 9 88.99 | 1 -7.82 | 0 1.00 05.00 | ш. | 0 |
| | | | | 235 | | | | | |

| | ATOM ATOM | 3931 3932 | N CD | PRO L PRO L | 120 120 | 31.018 30.919 | | | | 70.27 70.15 | L L | N C |
|----|--------------|--------------|------------|----------------|------------|------------------|---------|-----------|---------------------|----------------|--------|--------|
| | ATOM | 3933 | CA | | 120 | 29.871 | | | 1.00 | 71.14 | L | č |
| | MOTA | 3934 | CB | PRO L | | 29.149 | | | | 70.76 | L | C |
| 5 | ATOM | 3935 | CG | | 120 | 30.185 | | | | 70.81 | L | C |
| | ATOM | 3936 | C | PRO L | | 28.917 | | | | 71.90 72.28 | L L | C |
| | ATOM ATOM | 3937 3938 | N O | PRO L SER L | | 28.743 28.311 | | | | 73.49 | L | N |
| | ATOM | 3939 | CA | SER L | | 27.432 | | | | 75.09 | L | Ċ |
| 10 | ATOM | 3940 | CB | | 121 | 27.094 | | | | 75.12 | L | C |
| 10 | ATOM | 3941 | ŌĠ | SER L | | 26.586 | 85.86 | | 1.00 | 75.74 | L | 0 |
| | ATOM | 3942 | С | SER L | | 26.132 | | | 1.00 | 76.41 | L | C |
| | MOTA | 3943 | 0 | SER L | | 25.753 | | | | 76.22 | Ŀ | O |
| | ATOM | 3944 | N | SER L | | 25.406 | | | | 77.92 79.32 | L L | N C |
| 15 | ATOM | 3945 3946 | CA CB | SER L SER L | 122 | 24.027 23.326 | | | $\frac{1.00}{1.00}$ | 79.46 | L | C |
| | ATOM ATOM | 3947 | OG | SER L | | 24.063 | | | | 81.39 | L | ŏ |
| | ATOM | 3948 | Č | SER L | | 23.128 | | | | 79.71 | L | C |
| | ATOM | 3949 | 0 | SER L | 122 | 22.36 | | | 1.00 | 79.61 | L | 0 |
| 20 | ATOM | 3950 | N | GLU L | | 23.24 | | | | 79.84 | L | N |
| | ATOM | 3951 | CA | GLU L | | 22.35 | | | | 80.62 82.32 | L L | C |
| | MOTA | 3952 | CB | GLU L | | 22.642 21.47 | | | | 84.76 | L L | C |
| | ATOM ATOM | 3953 3954 | CG CD | GLU L | | 21.98 | | | | 86.63 | L | Č |
| 25 | ATOM | 3955 | OE1 | | | 21.54 | | | | 88.17 | L | 0 |
| | ATOM | 3956 | OE2 | GLU L | 123 | 22.83 | | | | 87.03 | L | 0 |
| | ATOM | 3957 | С | GLU L | | 22.34 | | | | 79.85 | L | C |
| | ATOM | 3958 | 0 | GLU L | | 21.29 | | | | 79.94 79.17 | L L | O N |
| 00 | MOTA | 3959 3960 | N | GLN L GLN L | | 23.486 23.628 | | | | 78.84 | L | C |
| 30 | ATOM ATOM | 3960 | CA CB | GLN L | | 25.11 | | | 1.00 | 77.47 | L | č |
| | ATOM | 3962 | CG | GLN L | | 25.59 | | | 1.00 | 75.52 | L | С |
| | MOTA | 3963 | CD | GLN L | 124 | 27.16 | | | 1.00 | | L | C |
| | MOTA | 3964 | OE1 | | | 27.73 | | | | 75.06 | L L | N |
| 35 | MOTA | 3965 3966 | NE2 C | GLN L | | 27.81 23.22 | | | | 74.95 79.38 | L | C |
| | MOTA ATOM | 3967 | 0 | GLN L | | 22.71 | | | | 78.57 | L | ŏ |
| | ATOM | 3968 | Ň | LEU L | | 23.53 | | 7 -4.708 | 1.00 | 80.14 | L | N |
| | MOTA | 3969 | CA | LEU L | | 23.19 | | | | 80.82 | L | C |
| 40 | MOTA | 3970 | CB | LEU L | | 23.62 | | | | | Ŀ | C |
| | ATOM | 3971 | CG | LEU L | | 24.77 25.49 | | | | 78.76 78.25 | L L | C |
| | MOTA MOTA | 3972 3973 | | LEU L | 125 | 25.49 | | | | | L | č |
| | ATOM | 3974 | CDZ | | 125 | 21.67 | | | | 81.71 | L | Ċ |
| 45 | ATOM | 3975 | ŏ | | 125 | 21.22 | 2 90.37 | 2 -2.956 | | 82.15 | L | 0 |
| | MOTA | 3976 | N | THR L | | 20.89 | | | | 81.94 | Ŀ | N |
| | MOTA | 3977 | CA | THR L | | 19.47 | | | | 82.43 | Ŀ | C |
| | ATOM | 3978 | CB OC1 | THR L | | 18.74 19.10 | | | | 82.87 84.01 | L L | C |
| 50 | ATOM ATOM | 3979 3980 | OG1 CG2 | | | 19.11 | | | | 83.71 | L | č |
| 30 | ATOM | 3981 | C | THR L | | 19.18 | | | | 82.03 | Ŀ | C |
| | MOTA | 3982 | 0 | THR L | | 18.21 | 8 89.26 | | | 83.16 | L | 0 |
| | MOTA | 3983 | N | SER L | | 19.97 | | | | 81.29 | L | N |
| | ATOM | 3984 | CA | SER L | | 19.76 | | | | 80.30 81.26 | L L | C |
| 55 | MOTA MOTA | 3985 3986 | CB OG | SER L SER L | | 20.70 20.07 | | | | 82.17 | L | Õ |
| | ATOM | 3987 | C | SER L | | 19.95 | | | | 78.92 | L | Č |
| | ATOM | 3988 | ŏ | SER L | 127 | 19.47 | | | 1.00 | 79.15 | L | 0 |
| | MOTA | 3989 | N | GLY L | 128 | 20.66 | 1 89.13 | | | 77.27 | L | N |
| 60 | MOTA | 3990 | CA | GLY L | | 21.10 | | | | 76.66 | L | C |
| | ATOM | 3991 | C | GLY L | | 22.57 | | | | 76.00 75.56 | L L | C 0 |
| | MOTA | 3992 | O M | GLY L GLY L | | 22.94 23.39 | | | | 75.16 | L L | N |
| | MOTA ATOM | 3993 3994 | N CA | GLY L | | 24.79 | | | | 73.79 | L | Ĉ |
| 65 | ATOM | 3995 | C | GLY L | 129 | 25.75 | 0 89.16 | 51 -0.515 | 1.00 | 72.59 | L | С |
| | ATOM | 3996 | 0 | GLY L | 129 | 25.39 | 1 89.35 | 50 -1.659 | 1.00 | 71.66 | Ŀ | 0 |
| | ATOM | 3997 | N | ALA L | | 26.97 | | | | 71.12 | L | N |
| | ATOM | 3998 | CA | ALA L | | 27.99 | | | | 69.78 69.16 | L L | C |
| | MOTA | 3999 | CB | ALA L | T20 | 28.26 | J J1.48 | ٠٥.۶٥١ عر | . 1.00 | 07.10 | | C |

| | | | | | | | | | _ | | _ |
|-----|--------------|--------------|--------------------------------|-----|------------------|------------------|------------------|--------------------------|--------|----------|--------|
| | MOTA | 4000 C | | 29. | 248 | 88.975 | -0.726 0.402 | 1.00 69.14 1.00 69.40 | L L | | C O |
| | ATOM | 4001 C | 404 | | 693 685 | 89.059 88.053 | -1.568 | 1.00 67.83 | L | | И |
| | ATOM | 4002 N | N SER L 131 CA SER L 131 | | 954 | 87.324 | -1.317 | 1.00 66.38 | L | | С |
| 5 | ATOM ATOM | | CB SER L 131 | | 761 | 85.779 | -1.366 | 1.00 66.45 | L | | C |
| 5 | MOTA | | OG SER L 131 | | 911 | 85.269 | -0.267 | 1.00 65.95 | L L | | C 0 |
| | ATOM | | C SER L 131 | | .977 | 87.774 | -2.347 -3.602 | 1.00 65.46 1.00 65.33 | L | | 0 |
| | MOTA | | SER L 131 | | .640 .141 | 87.847 88.177 | -1.850 | 1.00 64.00 | Ĺ | | N |
| | ATOM | | N VAL L 132 CA VAL L 132 | | .236 | 88.632 | -2.718 | 1.00 63.13 | L | | C |
| 10 | ATOM ATOM | | CA VAL L 132 CB VAL L 132 | | 819 | 89.972 | -2.286 | 1.00 63.18 | L | | C |
| | ATOM | 4011 | CG1 VAL L 132 | 35 | .786 | 90.546 | -3.235 | 1.00 62.10 | L | | C C |
| | MOTA | 4012 | CG2 VAL L 132 | | .797 | 90.979 | -2.012 -2.681 | 1.00 63.46 1.00 62.52 | L L | | C |
| | MOTA | | C VAL L 132 | | .287 .689 | 87.545 87.053 | -1.599 | 1.00 61.71 | Ŀ | | ō |
| 15 | ATOM | | O VAL L 132 N VAL L 133 | | .674 | 87.092 | -3.864 | 1.00 62.28 | L | | N |
| | MOTA MOTA | | N VAL L 133 CA VAL L 133 | | .508 | 85.922 | -4.004 | 1.00 61.13 | L | | C |
| | ATOM | | CB VAL L 133 | | .845 | 84.812 | -4.879 | 1.00 60.79 | L | | C |
| | ATOM | 4018 | CG1 VAL L 133 | | .666 | 83.560 | -4.734 | 1.00 61.21 1.00 60.87 | L L | | C |
| 20 | MOTA | | CG2 VAL L 133 | | .490 .779 | 84.536 86.296 | -4.496 -4.687 | 1.00 60.84 | Ī | | Č |
| | MOTA | | C VAL L 133 O VAL L 133 | | .838 | 87.026 | -5.766 | 1.00 59.39 | I | , | 0 |
| | MOTA MOTA | | O VAL L 133 N CYS L 134 | | .808 | 85.738 | -4.151 | 1.00 60.55 | I. | | N |
| | ATOM | | CA CYS L 134 | | .170 | 85.866 | -4.711 | 1.00 60.80 | I I | | C |
| 25 | ATOM | | C CYS L 134 | | .910 | 84.507 | -4.875 | 1.00 58.83 1.00 58.54 | I | | Ö |
| | ATOM | | O CYS L 134 | | .022 | 83.716 86.783 | -3.947 -3.760 | 1.00 50.34 | ī | | Č |
| | ATOM | | CB CYS L 134 SG CYS L 134 | | .525 | 87.373 | -4.465 | 1.00 66.69 | I | , | S |
| | ATOM ATOM | 4027 4028 | SG CYS L 134 N PHE L 135 | | .465 | 84.202 | -6.034 | 1.00 58.10 | Ī | | N |
| 30 | ATOM | 4029 | CA PHE L 135 | 42 | .320 | 83.024 | -6.337 | 1.00 58.00 | I | | C |
| | MOTA | 4030 | CB PHE L 135 | | 916 | 82.231 | -7.608 7.504 | 1.00 57.99 1.00 59.98 | I | | C |
| | MOTA | 4031 | CG PHE L 135 | |).563).199 | 81.667 80.894 | -7.504 -6.353 | 1.00 60.26 | Ī | | Č |
| | ATOM | 4032 | CD1 PHE L 135 CD2 PHE L 135 | |).570 | 81.927 | -8.426 | 1.00 60.52 | | | С |
| 95 | MOTA | 4033 4034 | CD2 PHE L 135 CE1 PHE L 135 | | 3.918 | 80.414 | -6.220 | 1.00 60.79 | | | C |
| 35 | MOTA MOTA | 4035 | CE2 PHE L 135 | | 3.274 | 81.405 | -8.208 | 1.00 60.24 | | _ | C |
| | ATOM | 4036 | CZ PHE L 135 | | 7.979 | 80.723 | -7.131 | 1.00 60.17 1.00 57.37 | | L L | C |
| | ATOM | 4037 | C PHE L 135 | | 3.695 | 83.390 84.430 | -6.360 -6.793 | 1.00 57.37 | | _ | ŏ |
| | MOTA | 4038 | O PHE L 135 N LEU L 136 | | 1.065 1.475 | 82.615 | -5.732 | 1.00 56.20 | | <u>.</u> | N |
| 40 | MOTA | 4039 4040 | N LEU L 136 CA LEU L 136 | | 5.902 | 82.636 | -5.797 | 1.00 56.01 | | Ŀ | C |
| | MOTA ATOM | 4041 | CB LEU L 136 | | 5.466 | 82.926 | -4.349 | 1.00 55.00 | | L | C |
| | MOTA | 4042 | CG LEU L 136 | | 5.197 | 84.380 | -3.849 | 1.00 53.48 1.00 52.57 | | L L | c |
| | MOTA | 4043 | CD1 LEU L 136 | | 4.809 | 84.348 84.588 | -3.487 -2.663 | 1.00 53.68 | | L | Č |
| 45 | MOTA | 4044 | CD2 LEU L 136 C LEU L 136 | | 7.206 6.461 | 81.270 | -6.220 | 1.00 55.46 | : | L | С |
| | MOTA | 4045 4046 | C LEU L 136 O LEU L 136 | | 6.648 | 80.361 | -5.363 | 1.00 55.72 | | L | 0 |
| | ATOM ATOM | 4047 | N ASN L 137 | 4 | 6.696 | 81.125 | -7.504 | 1.00 54.71 | | L | N |
| | ATOM | 4048 | CA ASN L 137 | | 6.908 | 79.853 | -8.217 -9.315 | 1.00 54.02 1.00 53.13 | | L L | C |
| 50 | MOTA | 4049 | CB ASN L 137 | | 5.912 4.576 | 79.848 79.532 | -8.824 | 1.00 54.07 | | L | Č |
| | MOTA | 4050 | CG ASN L 137 OD1 ASN L 137 | | 3.611 | | -9.556 | 1.00 54.87 | | L | 0 |
| | ATOM ATOM | 4051 4052 | ND2 ASN L 137 | | 4.486 | | -7.490 | 1.00 53.36 | | L - | N |
| | MOTA | 4053 | C ASN L 137 | | 8.280 | | | | | L L | C |
| 55 | ATOM | 4054 | O ASN L 137 | | 9.023 | | | | | P P | И |
| | MOTA | 4055 | N ASN L 138 | | 8.717 | | | | | L | Ĉ |
| | ATOM | 4056 | CA ASN L 138 CB ASN L 138 | | 0.019 9.948 | | | 1.00 53.07 | | L | С |
| | MOTA | 4057 4058 | CB ASN L 138 CG ASN L 138 | | 8.845 | 76.761 | -10.939 | 1.00 53.90 | | L | C |
| 60 | MOTA MOTA | 4059 | OD1 ASN L 138 | 4 | 7.738 | 77.168 | -11.022 | 1.00 54.05 | | Ŀ | O |
| JU | MOTA | 4060 | ND2 ASN L 138 | | 9.164 | | -11.148 | | | L L | C N |
| | MOTA | 4061 | C ASN L 138 | | 1.282 | | | | | r r | Ö |
| | MOTA | 4062 | O ASN L 138 | | 52.085 51.493 | | | | | L | N |
| 0.5 | MOTA | 4063 | N PHE L 139 CA PHE L 139 | | 2.686 | | | 1.00 50.60 | | L | C |
| 65 | MOTA MOTA | 4064 | CB PHE L 139 | | 2.243 | 80.105 | -5.715 | 1.00 50.74 | | Ŀ | C |
| | MOTA | 4066 | CG PHE L 139 | 5 | 51.351 | 79.679 | | | | L L | C |
| | MOTA | 4067 | CD1 PHE L 139 | | 51.889 | | | | | L | C |
| | MOTA | 4068 | CD2 PHE L 139 | ž | 50.020 | 79.854 | : ~4.JI: | , 1.00 -1.01 | | | _ |
| | | | | | 227 | | | | | | |

| | ATOM ATOM | 4069 4070 | CE1 PHE L 139 CE2 PHE L 139 | 49.1 | .53 | 78.832 79.655 | -2.264 -3.432 | 1.00 44.38 1.00 46.99 | L L | C C C |
|----|--------------|---------------------|--------------------------------|--------|--------------------|------------------|-----------------------|--------------------------|--------|--------------|
| | ATOM | $\frac{4071}{4072}$ | CZ PHE L 139 C PHE L 139 | | | 79.145 78.035 | -2.293 -5.987 | 1.00 46.10 1.00 50.74 | L L | C |
| 5 | ATOM ATOM | 4073 | O PHE L 139 | | | 76.992 | -5.659 | 1.00 51.42 | L | 0 |
| • | ATOM | 4074 | N TYR L 140 | | | 78.307 | -5.712 | 1.00 50.69 | L | Ŋ |
| | MOTA | 4075 | CA TYR L 140 | | | 77.532 | -4.737 | 1.00 51.02 | L | C |
| | ATOM | 4076 | CB TYR L 140 CG TYR L 140 | | | 76.384 75.429 | -5.565 -4.718 | 1.00 50.21 1.00 50.51 | L L | C |
| 10 | MOTA MOTA | 4077 4078 | CG TYR L 140 CD1 TYR L 140 | | | 75.776 | -4.260 | 1.00 50.90 | L | č |
| 10 | ATOM | 4079 | CE1 TYR L 140 | | | 74.860 | -3.430 | 1.00 51.73 | L | C |
| | MOTA | 4080 | CD2 TYR L 140 | | | 74.231 | -4.313 | 1.00 50.29 | L | C |
| | MOTA | 4081 | CE2 TYR L 140 | | | 73.398 | -3.442 | 1.00 49.97 | L | C |
| | ATOM | 4082 | CZ TYR L 140 | | | 73.731 72.903 | -3.033 -2.208 | 1.00 50.71 1.00 51.28 | L L | С О |
| 15 | ATOM ATOM | 4083 4084 | OH TYR L 140 C TYR L 140 | | | 78.436 | -4.108 | 1.00 52.40 | L | č |
| | ATOM | 4085 | O TYR L 140 | | | 79.318 | -4.849 | 1.00 53.02 | r . | O |
| | MOTA | 4086 | N PRO L 14: | | 914 | 78.189 | -2.837 | 1.00 53.24 | L | N |
| | MOTA | 4087 | CD PRO L 143 | | | 78.906 | -2.277 | 1.00 53.94 | L | C |
| 20 | ATOM | 4088 | CA PRO L 14: | | | 77.114 77.042 | -1.909 -0.809 | 1.00 53.82 1.00 54.17 | L L | C |
| | MOTA | 4089 4090 | CB PRO L 14: CG PRO L 14: | | | 78.417 | -0.809 | 1.00 54.65 | L | Č |
| | MOTA MOTA | 4090 | C PRO L 14: | | | 77.398 | -1.338 | 1.00 55.01 | L | C |
| | ATOM | 4092 | O PRO L 14: | | | 78.370 | -1.550 | 1.00 54.05 | L | 0 |
| 25 | MOTA | 4093 | N LYS L 14 | | | 76.460 | -0.588 | 1.00 56.78 | L | N |
| | ATOM | 4094 | CA LYS L 14 | | | 76.616 75.335 | -0.029 0.800 | 1.00 58.31 1.00 59.20 | L L | C |
| | MOTA MOTA | 4095 4096 | CB LYS L 14: CG LYS L 14: | | | 75.335 75.266 | 2.059 | 1.00 53.20 | L | č |
| | ATOM | 4097 | CD LYS L 14 | | | 74.381 | 3.213 | 1.00 66.39 | L | C |
| 30 | ATOM | 4098 | CE LYS L 14 | 2 53. | | 72.900 | 2.888 | 1.00 68.80 | L | C |
| | MOTA | 4099 | NZ LYS L 14 | | | 72.069 | 3.031 | 1.00 71.04 | L | N |
| | ATOM | 4100 | C LYS L 14 | | | 77.846 78.219 | 0.910 1.053 | 1.00 57.77 1.00 56.47 | L L | C |
| | ATOM ATOM | $\frac{4101}{4102}$ | O LYS L 14 N ASP L 14 | | | 78.301 | 1.647 | 1.00 58.64 | Ŀ | N |
| 35 | ATOM | 4102 | CA ASP L 14 | | | 79.452 | 2.544 | 1.00 60.59 | L | C |
| 00 | ATOM | 4104 | CB ASP L 14 | 3 54. | | 79.662 | 3.435 | 1.00 63.72 | L | C |
| | ATOM | 4105 | CG ASP L 14 | | | 78.208 | 3.881 | 1.00 68.11 | L | C |
| | ATOM | 4106 | OD1 ASP L 14 | | | 77.551 77.589 | 4.678 3.350 | 1.00 71.23 1.00 68.52 | L L | 0 |
| 40 | ATOM ATOM | 4107 4108 | OD2 ASP L 14 C ASP L 14 | | | 80.707 | 1.777 | 1.00 59.86 | Ŀ | Č |
| 40 | ATOM | 4109 | O ASP L 14 | | | 81.100 | 0.832 | 1.00 59.91 | L | 0 |
| | MOTA | 4110 | N ILE L 14 | | | 81.227 | 2.139 | 1.00 59.20 | Ŀ | N |
| | MOTA | 4111 | CA ILE L 14 | | | 82.460 | 1.579 | 1.00 57.84 | L L | C |
| 4 | ATOM | 4112 | CB ILE L 14 | | 848 495 | 82.198 81.527 | $0.240 \\ 0.333$ | 1.00 57.69 1.00 57.29 | Г Г | C |
| 45 | ATOM ATOM | $\frac{4113}{4114}$ | CG2 ILE L 14 CG1 ILE L 14 | | 459 | 83.396 | -0.447 | 1.00 56.97 | L | Č |
| | ATOM | 4115 | CD1 ILE L 14 | | 218 | 82.952 | -1.999 | 1.00 58.74 | L | C |
| | ATOM | 4116 | C ILE L 14 | | 517 | 83.183 | 2.516 | 1.00 57.84 | Ŀ | C |
| | ATOM | 4117 | O ILE L 14 | | 025 | 82.633 | 3.447 | 1.00 57.82 | L L | N |
| 50 | ATOM | 4118 4119 | N ASN L 14 CA ASN L 14 | | 398 474 | 84.459 85.216 | 2.352 3.173 | 1.00 58.32 1.00 58.90 | L | C |
| | MOTA MOTA | 4120 | CA ASN L 14 CB ASN L 14 | | 180 | 85.973 | 4.384 | 1.00 61.33 | L | C |
| | MOTA | 4121 | CG ASN L 14 | 5 50. | 711 | 84.960 | 5.438 | 1.00 65.53 | L | С |
| | MOTA | 4122 | OD1 ASN L 14 | | 064 | 84.629 | 6.562 | 1.00 67.50 | L | O |
| 55 | MOTA | 4123 | ND2 ASN L 14 | | 803 | 84.324 | 5.035 2.315 | 1.00 67.78 1.00 58.33 | L L | C N |
| | MOTA | 4124 | C ASN L 14 O ASN L 14 | | 750 351 | 86.163 86.782 | 1.573 | 1.00 57.41 | Ŀ | ō |
| | ATOM ATOM | 4125 4126 | O ASN L 14 N VAL L 14 | | 43.8 | 86.226 | 2.478 | 1.00 57.86 | L | \mathbf{N} |
| | ATOM | 4127 | CA VAL L 14 | | 555 | 87.234 | 1.924 | 1.00 58.06 | L | С |
| 60 | MOTA | 4128 | CB VAL L 14 | 6 45. | 303 | 86.517 | 1.079 | 1.00 57.95 | L | C |
| | ATOM | 4129 | CG1 VAL L 14 | | 307 | 86.211 87.508 | 1.872 0.160 | 1.00 57.78 1.00 58.46 | L L | C |
| | MOTA MOTA | $4130 \\ 4131$ | CG2 VAL L 14 C VAL L 14 | | 67 <u>4</u> 900 | 88.252 | 2.910 | 1.00 57.64 | Ŀ | C |
| | MOTA | 4132 | O VAL L 14 | | 598 | 87.920 | 4.076 | 1.00 58.21 | L | 0 |
| 65 | MOTA | 4133 | N ALA L 14 | .7 45. | 671 | 89.436 | 2.420 | 1.00 57.33 | L | N |
| | MOTA | 4134 | CA ALA L 14 | | 064 | 90.601 | 3.176 | 1.00 57.71 | L | C |
| | MOTA | 4135 | CB ALA L 14 | | .137 .014 | 91.686 91.255 | 3.585 2.324 | 1.00 55.87 1.00 57.31 | L L | C |
| | MOTA MOTA | 4136 4137 | C ALA L 14 | | .223 | 91.499 | $\frac{2.324}{1.101}$ | 1.00 57.31 | L | ŏ |
| | AIOM | 477/ | O 2002 11 15 | ., | | | | | | |

| | ATOM | 4138 | N TRP L 148 | | 91.453 | 2.894 2.236 | 1.00 57.87 1.00 58.89 | L L | N C |
|----|--------------|---------------------|--------------------------------|----------|--------------------|------------------|--------------------------|---------------------|--------|
| | ATOM ATOM | 4139 4140 | CA TRP L 148 CB TRP L 148 | | 92.218 91.584 | 2.236 | 1.00 57.33 | L | C |
| | MOTA | 4141 | CG TRP L 148 | 40.288 | 90.291 | 1.853 | 1.00 57.66 | L | C |
| 5 | ATOM | 4142 | CD2 TRP L 148 | | 90.085 | 0.541 | 1.00 57.55 | L L | C |
| | ATOM | $\frac{4143}{4144}$ | CE2 TRP L 148 CE3 TRP L 148 | | 88.685 90.945 | 0.329 -0.454 | 1.00 57.15 1.00 56.56 | F. | C |
| | ATOM ATOM | 4145 | CD1 TRP L 148 | | 89.005 | 2.371 | 1.00 58.03 | L | č |
| | MOTA | 4146 | NE1 TRP L 148 | 40.157 | 88.010 | 1.528 | 1.00 57.48 | L | N |
| 10 | MOTA | 4147 | CZ2 TRP L 148 | | 88.187 | -0.854 | 1.00 56.94 | L L | C |
| | ATOM ATOM | 4148 4149 | CZ3 TRP L 148 CH2 TRP L 148 | | 90.449 89.052 | -1.634 -1.835 | 1.00 57.22 1.00 57.66 | Ŀ | C |
| | ATOM | 4150 | C TRP L 148 | | 93.669 | 2.705 | 1.00 59.68 | L | Č |
| | ATOM | 4151 | O TRP L 148 | 42.073 | 93.972 | 3.876 | 1.00 58.38 | L | 0 |
| 15 | MOTA | 4152 | N LYS L 149 | | 94.576 | 1.727 | 1.00 60.92 1.00 62.70 | L L | N C |
| | MOTA ATOM | 4153 4154 | CA LYS L 149 CB LYS L 149 | | 95.970 96.770 | $2.071 \\ 1.601$ | 1.00 62.70 1.00 62.73 | L | c |
| | ATOM | 4155 | CG LYS L 149 | | 96.275 | 2.216 | 1.00 65.79 | L | C |
| | ATOM | 4156 | CD LYS L 149 | 45.191 | 97.199 | 1.883 | 1.00 67.30 | ŗ | C |
| 20 | MOTA | 4157 | CE LYS L 149 | | 97.132 | 2.928 2.346 | 1.00 68.06 1.00 69.75 | L L | C N |
| | MOTA MOTA | 4158 4159 | NZ LYS L 149 C LYS L 149 | | 97.631 96.513 | 1.393 | 1.00 69.75 1.00 64.55 | L L | C |
| | ATOM | 4160 | O LYS L 149 | | 96.480 | 0.179 | 1.00 65.43 | L | Ö |
| | ATOM | 4161 | N ILE L 150 | 39.297 | 96.975 | 2.238 | 1.00 66.29 | L | N |
| 25 | MOTA | 4162 | CA ILE L 150 | | 97.649 97.082 | $1.709 \\ 2.420$ | 1.00 68.24 1.00 67.61 | r L | C |
| | MOTA MOTA | 4163 4164 | CB ILE L 150 | | 97.148 | 1.483 | 1.00 66.74 | L | C |
| | ATOM | 4165 | CG1 ILE L 150 | | 95.617 | 2.807 | 1.00 68.87 | ${f L}$ | C |
| | ATOM | 4166 | CD1 ILE L 150 | | 94.846 | 2.900 | 1.00 68.94 | ŗ | C |
| 30 | MOTA | 4167 | C ILE L 150 | | 99.155 99.651 | 1.961 3.048 | 1.00 69.93 1.00 70.68 | L L | C |
| | ATOM ATOM | 4168 4169 | O ILE L 150 N ASP L 151 | | 99.893 | 0.919 | 1.00 70.00 | L | Ŋ |
| | MOTA | 4170 | CA ASP L 15 | 38.698 | 101.335 | 1.080 | 1.00 75.11 | L | C |
| | ATOM | 4171 | CB ASP L 15 | | | 1.563 | 1.00 76.60 | Ŀ | C |
| 35 | ATOM | 4172 | CG ASP L 15 | | 102.376 102.148 | 0.400 -0.744 | 1.00 78.00 1.00 80.12 | L L | C O |
| | ATOM ATOM | 4173 4174 | OD1 ASP L 15: OD2 ASP L 15: | | 102.148 | 0.660 | 1.00 30.12 | r r | ŏ |
| | ATOM | 4175 | C ASP L 15 | | 101.714 | 2.116 | 1.00 76.27 | L | C |
| | ATOM | 4176 | O ASP L 15 | 1 39.501 | 102.350 | 3.129 | 1.00 77.76 | L | 0 |
| 40 | ATOM | 4177 | N GLY L 15 | | | $1.858 \\ 2.684$ | 1.00 76.18 1.00 77.99 | L L | N C |
| | ATOM ATOM | 4178 4179 | CA GLY L 15. C GLY L 15. | | | 3.858 | 1.00 77.55 | L | č |
| | ATOM | 4180 | O GLY L 15 | 2 43.497 | 100.184 | 4.043 | 1.00 80.56 | L | 0 |
| | MOTA | 4181 | N SER L 15 | | 100.501 | 4.688 | 1.00 79.95 | $\mathbf{L}_{_{1}}$ | N |
| 45 | MOTA | 4182 | CA SER L 15 | | 99.673 100.083 | 5.878 6.931 | 1.00 80.24 1.00 79.86 | L L | C |
| | MOTA MOTA | 4183 4184 | CB SER L 15 OG SER L 15 | | 100.005 | 6.336 | 1.00 80.56 | Ŀ | ŏ |
| | MOTA | 4185 | C SER L 15 | 3 41.397 | 98.186 | 5.554 | 1.00 80.28 | L | C |
| | MOTA | 4186 | O SER L 15 | 3 40.625 | | 4.697 | 1.00 79.92 | L | O |
| 50 | MOTA | 4187 | N GLU L 15 CA GLU L 15 | | | 6.271 6.217 | 1.00 80.81 1.00 82.01 | L L | N C |
| | ATOM ATOM | 4188 4189 | CA GLU L 15 CB GLU L 15 | | | 7.000 | 1.00 82.58 | L | C |
| | ATOM | 4190 | CG GLU L 15 | 4 43.693 | 93.986 | 6.909 | 1.00 83.88 | L | C |
| | MOTA | 4191 | CD GLU L 15 | 4 44.934 | | 7.710 | 1.00 85.00 1.00 86.24 | L L | C O |
| 55 | MOTA | 4192 4193 | OE1 GLU L 15 OE2 GLU L 15 | | | 8.011 7.989 | 1.00 85.24 | Ŀ | Ö |
| | ATOM ATOM | 4194 | C GLU L 15 | | | 6.889 | 1.00 82.30 | L | Ċ |
| | ATOM | 4195 | O GLU L 15 | 4 40.455 | 95.942 | 7.884 | 1.00 81.97 | L | 0 |
| | MOTA | 4196 | N ARG L 15 | | | 6.220 | 1.00 82.65 1.00 83.03 | L L | N C |
| 60 | ATOM | 4197 4198 | CA ARG L 15 CB ARG L 15 | | | 6.761 5.785 | 1.00 83.03 | r L | C |
| | MOTA MOTA | 4198 | CG ARG L 15 | | | 6.190 | 1.00 84.92 | L | C |
| | ATOM | 4200 | CD ARG L 15 | 5 36.200 | 93.337 | 7.238 | 1.00 86.77 | L | C |
| | MOTA | 4201 | NE ARG L 15 | | | 7.153 7.146 | 1.00 88.25 1.00 88.42 | L L | N C |
| 65 | MOTA | 4202 4203 | CZ ARG L 15 NH1 ARG L 15 | | | 7.146 7.274 | 1.00 88.42 | P P | N |
| | MOTA ATOM | 4203 | NH2 ARG L 15 | | | 6.998 | 1.00 89.76 | L | N |
| | MOTA | 4205 | C ARG L 15 | 5 40.140 | 92.075 | 7.077 | 1.00 82.99 | L | C |
| | MOTA | 4206 | O ARG L 15 | 5 41.035 | 91.596 | 6.322 | 1.00 83.97 | L | 0 |

| | ATOM ATOM | 4207 4208 4209 | N GLN L 156 CA GLN L 156 CB GLN L 156 | 39.666 39.811 40.770 | 91.490 90.083 90.099 | 8.196 8.655 9.830 | 1.00 81.99 1.00 80.76 1.00 80.72 | L L L | C C |
|----|------------------------------|----------------------|---|----------------------------|----------------------------|----------------------------|--|-------------|---------------|
| 5 | ATOM ATOM ATOM ATOM | 4210 4211 4212 | CG GLN L 156 CD GLN L 156 OE1 GLN L 156 | 42.232 43.078 42.765 | 90.228 90.931 92.026 | 9.421 10.427 10.846 | 1.00 80.80 1.00 82.05 1.00 82.80 | L L L | с с с |
| | ATOM ATOM ATOM | 4213 4214 4215 | NE2 GLN L 156 C GLN L 156 O GLN L 156 | 44.169 38.459 38.334 | 90.282 89.288 88.061 | 10.857 8.952 8.733 | 1.00 82.66 1.00 80.18 1.00 80.18 | L L L | O C N |
| 10 | ATOM ATOM ATOM | 4216 4217 4218 | N ASN L 157 CA ASN L 157 CB ASN L 157 | 37.435 36.109 35.300 | 90.015 89.487 90.700 | 9.341 9.547 10.075 | 1.00 78.71 1.00 77.03 1.00 78.97 | L L L | C C |
| 15 | ATOM ATOM ATOM | 4219 4220 4221 | CG ASN L 157 OD1 ASN L 157 ND2 ASN L 157 | 33.882 33.573 33.032 | 90.323 89.132 91.339 | 10.592 10.652 10.954 | 1.00 80.56 1.00 82.32 1.00 81.05 | L L L | C O . N |
| | ATOM ATOM ATOM | 4222 4223 4224 | C ASN L 157 O ASN L 157 N GLY L 158 | 35.380 34.967 35.103 | 88.982 89.810 87.642 | 8.298 7.408 8.222 | 1.00 74.78 1.00 75.06 1.00 71.80 | r r r | 0 N |
| 20 | ATOM ATOM ATOM | 4225 4226 4227 | CA GLY L 158 C GLY L 158 O GLY L 158 | 34.183 35.024 34.664 | 87.163 86.671 86.616 | 7.173 6.129 4.978 | 1.00 67.26 1.00 65.35 1.00 65.64 | L L | 0 0 |
| | ATOM ATOM ATOM | 4228 4229 4230 | N VAL L 159 CA VAL L 159 CB VAL L 159 | 36.203 37.256 38.648 | 86.316 85.881 86.582 | 6.524 5.623 5.757 | 1.00 62.86 1.00 60.58 1.00 60.31 | L L | N C C |
| 25 | MOTA ATOM MOTA | 4231 4232 4233 | CG1 VAL L 159 CG2 VAL L 159 C VAL L 159 | 39.725 38.678 37.506 | 85.978 88.045 84.421 | 4.872 5.438 5.903 | 1.00 57.65 1.00 59.05 1.00 59.71 | L L L | 0 0 0 |
| 30 | ATOM ATOM ATOM | 4234 4235 4236 | O VAL L 159 N LEU L 160 CA LEU L 160 | 37.844 37.374 37.557 | 83.995 83.625 82.157 | 7.023 4.863 4.890 | 1.00 60.16 1.00 57.40 1.00 55.89 | L L L | O N C |
| | MOTA MOTA MOTA | 4237 4238 4239 | CB LEU L 160 CG LEU L 160 CD1 LEU L 160 | 36.153 35.473 34.081 | 81.523 81.481 80.756 | 4.887 6.386 6.541 | 1.00 55.19 1.00 55.02 1.00 52.85 | L L L | . C C |
| 35 | MOTA ATOM ATOM | 4240 4241 4242 | CD2 LEU L 160 C LEU L 160 O LEU L 160 | 36.367 38.467 38.156 | 80.947 81.698 81.965 | 7.670 3.747 2.593 | 1.00 51.54 1.00 54.28 1.00 54.43 | L L L | С О |
| | MOTA ATOM ATOM | 4243 4244 4245 | N ASN L 161 CA ASN L 161 CB ASN L 161 | 39.609 40.587 41.879 | 81.137 80.590 81.051 | 4.096 3.258 3.771 | 1.00 53.43 1.00 53.45 1.00 54.82 | L L L | N C C |
| 40 | MOTA MOTA MOTA | 4246 4247 4248 | CG ASN L 161 OD1 ASN L 161 ND2 ASN L 161 | 42.029 41.519 42.657 | 82.496 83.084 83.091 | 3.642 2.665 4.610 | 1.00 56.80 1.00 56.52 1.00 55.21 | L L L | 0 C |
| 45 | MOTA ATOM MOTA | 4249 4250 4251 | C ASN L 161 O ASN L 161 N SER L 162 | 40.734 40.319 41.253 | 79.081 78.384 78.571 | 3.176 4.043 2.016 | 1.00 53.57 1.00 53.48 1.00 53.97 | L L | О О С |
| | ATOM ATOM ATOM | 4252 4253 4254 | CA SER L 162 CB SER L 162 OG SER L 162 | 41.350 39.961 40.034 | 77.148 76.646 75.376 | 1.750 1.339 0.681 | 1.00 53.68 1.00 52.18 1.00 55.01 | L L | 0 0 0 |
| 50 | ATOM ATOM ATOM | 4255 4256 4257 | C SER L 162 O SER L 162 N TRP L 163 | 42.407 42.432 43.198 | 76.915 77.585 75.906 | 0.696 -0.222 0.853 | 1.00 54.09 1.00 55.23 1.00 53.72 | L L L | 0 N |
| | ATOM ATOM ATOM | 4258 4259 4260 | CA TRP L 163 CB TRP L 163 CG TRP L 163 | 44.378 45.659 46.120 | 75.589 75.480 76.734 | 0.150 1.064 1.597 | 1.00 54.51 1.00 57.00 1.00 59.37 | L L L | 0 0 0 |
| 55 | MOTA ATOM MOTA | 4261 4262 4263 | CD2 TRP L 163 CE2 TRP L 163 CE3 TRP L 163 | 45.511 46.278 44.475 | 77.432 78.524 77.121 | 2.684 2.950 3.538 | 1.00 59.95 1.00 61.25 1.00 60.81 | L L | C C |
| 60 | ATOM ATOM ATOM | 4264 4265 4266 | CD1 TRP L 163 NE1 TRP L 163 CZ2 TRP L 163 | 47.228 47.313 46.021 | 77.427 78.570 79.336 | 1.237 2.022 3.953 | 1.00 60.45 1.00 62.43 1.00 61.48 | L L | N C |
| | ATOM ATOM ATOM | 4267 4268 4269 | CZ3 TRP L 163 CH2 TRP L 163 C TRP L 163 | 44.208 44.941 44.152 | 77.956 79.117 74.125 | 4.536 4.659 -0.338 | 1.00 60.93 1.00 60.59 1.00 53.80 | L L | C C C |
| 65 | ATOM ATOM ATOM | 4270 4271 4272 | O TRP L 163 N THR L 164 CA THR L 164 | | 73.221 73.884 72.603 | 0.367 -1.511 -2.117 | 1.00 53.91 1.00 52.58 1.00 51.82 | L L L | С И О |
| | MOTA MOTA MOTA | 4273 4274 4275 | CB THR L 164 OG1 THR L 164 CG2 THR L 164 | 44.605 45.805 | 73.483 | -3.624 -4.091 -4.131 | 1.00 51.25 1.00 51.26 1.00 50.51 | L L L | С О С |

| | n u | | | | | | | _ | ~ |
|----|--------------|------------------|------------------------------|------------------|------------------|------------------|--------------------------|--------|------------|
| | MOTA | 4276 C | | 45.845 | 71.880 | -1.815 | 1.00 51.96 | L | C |
| | MOTA | 4277 O | | 46.712 | 72.419 | -1.359 | 1.00 52.00 1.00 53.05 | L L | И |
| | MOTA | 4278 N | | 45.971 | 70.649 | -2.208 -1.993 | 1.00 53.05 | L | C |
| | MOTA | 4279 C | | 47.165 | 69.837 68.360 | -1.999 | 1.00 55.45 | L | č |
| 5 | ATOM | 4280 C | | 46.799 46.252 | 67.855 | -0.542 | 1.00 60.07 | L | č |
| | ATOM | | G ASP L 165 | 45.044 | 67.725 | -0.411 | 1.00 61.03 | L | ō |
| | ATOM | | D1 ASP L 165 D2 ASP L 165 | 46.984 | 67.497 | 0.454 | 1.00 63.38 | L | Ö |
| | MOTA | | | 48.009 | 70.135 | -3.161 | 1.00 52.57 | L | |
| 40 | MOTA | 4284 C | | 47.508 | 70.595 | -4.165 | 1.00 52.07 | L | 0 |
| 10 | ATOM ATOM | 4285 O 4286 N | | 49.223 | 69.688 | -3.087 | 1.00 50.87 | L | N |
| | ATOM | | A GLN L 166 | 50.207 | 69.825 | -4.145 | 1.00 50.45 | L | |
| | ATOM | | B GLN L 166 | 51.473 | 69.184 | -3.640 | 1.00 49.06 | L | |
| | ATOM | | G GLN L 166 | 52.576 | 69.588 | -4.484 | 1.00 50.09 | L | |
| 15 | ATOM | | D GLN L 166 | 53.909 | 69.326 | -4.010 | 1.00 50.81 | L | |
| 15 | ATOM | | E1 GLN L 166 | 54.122 | 68.377 | -3.327 | 1.00 50.74 | L | |
| | ATOM | | JE2 GLN L 166 | 54.822 | 70.264 | -4.311 | 1.00 50.10 | L | |
| | ATOM | 4293 C | | 49.653 | 69.162 | -5.444 | 1.00 51.47 | L | |
| | ATOM | 4294 C | | 49.199 | 68.063 | -5.439 | 1.00 50.46 | Ŀ | |
| 20 | ATOM | 4295 N | | 49.577 | 69.901 | -6.493 | 1.00 52.11 | Ŀ | |
| | MOTA | | CA ASP L 167 | 49.257 | 69.421 | -7.799 | 1.00 54.31 | L | |
| | ATOM | | CB ASP L 167 | 49.503 | 70.542 | -8.785 | 1.00 56.80 | L | |
| | ATOM | | CG ASP L 167 | 48.910 | | -10.071 | 1.00 59.47 | L | |
| | MOTA | 4299 C | DD1 ASP L 167 | 47.643 | | -10.035 | 1.00 60.73 | L | |
| 25 | MOTA | 4300 0 | DD2 ASP L 167 | 49.615 | | -11.037 | 1.00 60.31 | L | |
| | ATOM | 4301 0 | | 50.249 | 68.275 | -8.167 | 1.00 55.01 | L | |
| | ATOM | | O ASP L 167 | 51.401 | 68.414 | -8.028 | 1.00 55.28 1.00 55.89 | L | |
| | MOTA | | N SER L 168 | 49.733 | 67.109 | -8.488 | 1.00 56.86 | I | |
| | MOTA | | CA SER L 168 | 50.473 | 65.926 | -9.062 -9.158 | 1.00 56.64 | ī | |
| 30 | MOTA | | CB SER L 168 | 49.570 | 64.627 | -9.138 -9.870 | 1.00 50.04 | Ī | |
| | MOTA | | OG SER L 168 | 48.456 51.220 | 65.012 | -10.403 | 1.00 56.36 | Ī | |
| | MOTA | | C SER L 168 | 52.027 | | -10.659 | 1.00 57.56 | Ī | |
| | MOTA | | O SER L 168 | 51.052 | | -11.101 | 1.00 56.30 | I | |
| | MOTA | | N LYS L 169 | 51.800 | 67.138 | -12.364 | 1.00 57.59 | Ī | |
| 35 | ATOM | | CA LYS L 169 CB LYS L 169 | 50.798 | 67.440 | -13.469 | 1.00 59.32 | I | |
| | ATOM | | CB LYS L 169 CG LYS L 169 | 49.678 | | -13.648 | 1.00 62.12 | I | |
| | MOTA | | CD LYS L 169 | 48.998 | | -15.020 | 1.00 62.52 | I | , C |
| | MOTA | | CE LYS L 169 | 48.225 | | -14.949 | 1.00 64.22 | Ι | , c |
| 40 | ATOM ATOM | | NZ LYS L 169 | 47.154 | | -16.011 | 1.00 63.95 | I | |
| 40 | ATOM | | C LYS L 169 | 52.812 | | -12.332 | 1.00 57.97 | I | |
| | ATOM | | O LYS L 169 | 53.946 | 68.201 | -12.490 | 1.00 57.97 | I | |
| | ATOM | | N ASP L 170 | 52.446 | | -11.987 | 1.00 57.59 | Ι | |
| | ATOM | | CA ASP L 170 | 53.438 | 70.868 | -11.910 | 1.00 57.49 | I | |
| 45 | ATOM | | CB ASP L 170 | 52.788 | 72.129 | -12.489 | 1.00 60.30 | I | |
| | ATOM | | CG ASP L 170 | 51.710 | | -11.564 | 1.00 62.68 | I | |
| | ATOM | | OD1 ASP L 170 | 51.622 | | -10.321 | 1.00 65.22 | I | |
| | MOTA | 4323 | OD2 ASP L 170 | 50.896 | | -12.024 | 1.00 62.99 | | |
| | MOTA | | C ASP L 170 | 53.901 | 71.148 | | 1.00 55.90 | | i C |
| 50 | MOTA | 4325 | O ASP L 170 | 54.694 | 72.062 | | 1.00 54.92 | | L O L N |
| | MOTA | | N SER L 171 | 53.446 | 70.339 | -9.478 | 1.00 54.19 1.00 53.65 | | r C |
| | MOTA | | CA SER L 171 | 54.038 | 70.455 | -8.108 | 1.00 53.65 | | r C |
| | MOTA | | CB SER L 171 | 55.440 | 70.037 | -8.123 | 1.00 54.70 | | L O |
| | MOTA | | OG SER L 171 | 55.708 | 68.799 | -8.882 | 1.00 52.81 | | r C |
| 55 | MOTA | | C SER L 171 | 53.876 | 71.866 | -7.423 | 1.00 52.51 | | L Ö |
| | MOTA | | O SER L 171 | 54.596 | 72.185 | -6.436 -7.840 | 1.00 51.64 | | L N |
| | MOTA | | N THR L 172 | 52.826 | 72.583 73.877 | -7.362 | 1.00 51.66 | | L C |
| | MOTA | | CA THR L 172 | 52.507 | 74.809 | -8.372 | 1.00 51.61 | | L C |
| | MOTA | 4334 | CB THR L 172 | 52.052 | 74.383 | | 1.00 50.22 | | L O |
| 60 | MOTA | 4335 | OG1 THR L 172 | 50.823 52.978 | 75.076 | | | | L Č |
| | ATOM | 4336 | CG2 THR L 172 | 52.978 | 73.740 | | | | L Č |
| | ATOM | 4337 | C THR L 172 | 50.672 | 72.688 | | | | L O |
| | ATOM | 4338 | O THR L 172 | 51.051 | 74.805 | | | | L N |
| 0. | MOTA | 4339 | N TYR L 173 CA TYR L 173 | 49.878 | | | | | L C |
| 65 | MOTA | 4340 4341 | CA TYR L 173 CB TYR L 173 | 50.334 | | | | | L C |
| | ATOM | $4341 \\ 4342$ | CG TYR L 173 | 51.209 | | | 1.00 52.92 | | L C |
| | ATOM ATOM | 4342 | CD1 TYR L 173 | 52.517 | | | 1.00 53.07 | | ь с |
| | ATOM | 4343 | CE1 TYR L 173 | 53.329 | | | | | L C |
| | WI OM | #J## | | | | | | | |

| | | | 50.703 73.175 -1.858 1.00 53.06 L C | |
|----|--------------|--|---|--|
| | MOTA MOTA | 4345 CD2 TYR L 173 4346 CE2 TYR L 173 | 51.564 72.130 -1.375 1.00 54.56 L C | |
| | ATOM ATOM | 4347 CZ TYR L 173 4348 OH TYR L 173 | 53.703 71.126 -1.149 1.00 56.41 L O | |
| 5 | ATOM ATOM | 4349 C TYR L 173 4350 O TYR L 173 | 48.987 75.983 3.173 1.00 52.51 L O N | |
| | MOTA | 4351 N SER L 174 | 47.778 75.895 -4.809 1.00 56.59 L C | |
| | ATOM ATOM | 4353 CB SER L 174 | 45.898 76.574 -6.002 1.00 56.89 | |
| 10 | MOTA | 4354 OG SER L 174 4355 C SER L 174 | 45.984 77.303 -3.506 1.00 57.56 L C | |
| | ATOM ATOM | 4356 O SER L 174 | 45.807 76.544 -2.616 1.00 56.52 L N | |
| | ATOM ATOM | 4357 N MET L 175 4358 CA MET L 175 | 44.637 78.939 -2.408 1.00 60.02 L C | |
| 15 | MOTA | 4359 CB MET L 175 | 45.288 81.039 -1.286 1.00 66.41 L C | |
| | MOTA MOTA | 4361 SD MET L 175 | 45.001 81.374 0.591 1.00 70.49 L S | |
| | MOTA | 4362 CE MET L 175 4363 C MET L 175 | 43.567 79.795 -2.863 1.00 59.29 L C | |
| 20 | ATOM ATOM | 4364 O MET L 175 | 43.680 80.541 -3.860 1.00 59.37 L N | |
| | ATOM ATOM | 4365 N SER L 176 4366 CA SER L 176 | 41.309 80.502 -2.491 1.00 59.10 L | |
| | MOTA | 4367 CB SER L 176 | 39 208 80.594 -2.947 1.00 60.69 L O | |
| 25 | MOTA MOTA | 4369 C SER L 176 | 40.964 81.310 -1.208 1.00 50.40 L O | |
| | MOTA MOTA | 4370 O SER L 176 4371 N SER L 177 | 40.659 82.616 -1.358 1.00 57.20 L N | |
| | MOTA | 4372 CA SER L 177 | 40.193 83.440 c.205 1.00 56.59 L C | |
| 30 | ATOM ATOM | 4374 OG SER L 177 | 40.940 85.208 1.304 1.00 55.06 II C | |
| 30 | MOTA | 4375 C SER L 177 4376 O SER L 177 | 38.889 84.030 0.133 1.00 60.67 L O | |
| | MOTA MOTA | 4377 N THR L 178 | 37.970 83.906 0.433 1.00 60.53 L C | |
| 35 | ATOM ATOM | 4378 CA THR L 178 4379 CB THR L 178 | 35.594 83.260 0.267 1.00 60.58 L C | |
| 35 | MOTA | 4380 OG1 THR L 178 | 34 146 83.762 -0.046 1.00 61.14 L C | |
| | MOTA MOTA | 4382 C THR L 178 | 36.127 85.364 1.530 1.00 62.36 II C | |
| | MOTA | 4383 O THR L 178 4384 N LEU L 179 | 35.820 86.606 1.189 1.00 64.02 L N | |
| 40 | MOTA MOTA | 4385 CA LEU L 179 | 35.321 87.641 2.073 1.00 66.01 L C | |
| | MOTA MOTA | 4386 CB LEU L 179 4387 CG LEU L 179 | 35.527 90.141 2.547 1.00 66.63 L C | |
| | MOTA | 4388 CD1 LEU L 179 | 35.694 89.990 4.055 1.00 66.81 L C | |
| 45 | MOTA MOTA | 4390 C LEU L 179 | 33.808 87.792 1.872 1.00 66.30 L O | |
| | MOTA | 4391 O LEU L 179 4392 N THR L 180 | 33.078 87.369 2.912 1.00 67.93 L N | |
| | MOTA MOTA | 4393 CA THR L 180 | 31.622 87.393 2.887 1.88 76.36 L C | |
| 50 | MOTA MOTA | 4394 CB THR L 180 4395 OG1 THR L 180 | 31.691 84.981 2.712 1.00 71.93 E C | |
| | ATOM | 4396 CG2 THR L 180 | 31.088 88.536 3.748 1.00 71.78 L C | |
| | MOTA MOTA | 4398 O THR L 180 | 31.298 88.594 4.951 1.00 71.49 L N | |
| 55 | ATOM ATOM | | 29.918 90.676 3.846 1.00 76.89 L C | |
| | ATOM | 4401 CB LEU L 181 | 30.347 91.926 3.632 1.00 76.56 L C | |
| | MOTA MOTA | 4403 CD1 LEU L 181 | 32.154 92.713 1.419 1.00 76.50 1.60 1.60 | |
| 60 | ATOM | 4404 CD2 LEU L 181 | 32.736 92.478 3.751 1.00 78.78 L C 28.381 90.605 4.016 1.00 78.78 L C | |
| | IOTA IOTA | 4406 O LEU L 181 | 27.828 89.535 4.105 1.00 80.37 L N | |
| | ATOL | | 26.289 91.915 3.858 1.00 82.33 L C | |
| 65 | | 4 4409 CB THR L 182 | 25.662 92.615 5.07 1.00 81.85 L O | |
| | ATO! ATO! | и 4411 CG2 THR L 182 | 25.240 91.514 6.082 1.00 82.04 L C | |
| | OTA | 4412 C THR L 182 | 26.237 92.856 2.623 1.00 84 91 L O | |
| | OTA | M 4413 O THR L 182 | 242 | |

| | ATOM ATOM | 4414 4415 | N LYS L 183 CA LYS L 183 | | 92.658 93.594 | 1.644 0.562 | 1.00 84.68 1.00 86.00 | L L | N C |
|-----|--------------|----------------|--------------------------------|--------------------|--------------------|------------------|--------------------------|--------------|--------|
| | MOTA | 4416 | CB LYS L 183 | 25.019 | 93.197 | -0.749 | 1.00 86.72 | L | C |
| _ | MOTA | 4417 | CG LYS L 183 | | 93.322 93.995 | -0.752 -2.073 | 1.00 86.54 1.00 87.47 | L L | C |
| 5 | ATOM ATOM | 4418 4419 | CD LYS L 183 CE LYS L 183 | | 93.785 | -2.691 | 1.00 88.10 | L | Č |
| | ATOM | 4420 | NZ LYS L 183 | | 94.811 | -3.743 | 1.00 89.02 | L | N |
| | MOTA | 4421 | C LYS L 183 | | 95.056 | 1.041 | 1.00 86.08 | L | С |
| | ATOM | 4422 | O LYS L 183 | | 96.024 | 0.508 | 1.00 86.38 | L | 0 |
| 10 | ATOM | 4423 | N ASP L 184 | | 95.158 96.437 | $2.167 \\ 2.721$ | 1.00 85.81 1.00 85.79 | L L | N C |
| | MOTA | 4424 4425 | CA ASP L 184 CB ASP L 184 | | 96.160 | 3.897 | 1.00 87.59 | L | Č |
| | MOTA MOTA | 4426 | CG ASP L 184 | | 97.349 | 4.851 | 1.00 89.93 | L | C |
| | ATOM | 4427 | OD1 ASP L 184 | | 98.440 | 4.386 | 1.00 90.99 | \mathbf{L} | 0 |
| 15 | MOTA | 4428 | OD2 ASP L 184 | | 97.125 | 6.059 | 1.00 91.11 | L | 0 C |
| | MOTA | 4429 | C ASP L 184 | | 97.177 98.391 | 3.133 2.998 | 1.00 84.86 1.00 85.11 | L L | 0 |
| | MOTA | $4430 \\ 4431$ | O ASP L 184 N GLU L 185 | | 96.403 | 3.685 | 1.00 83.36 | Ĺ | Ŋ |
| | MOTA MOTA | 4431 | CA GLU L 185 | | 96.852 | 4.008 | 1.00 82.20 | L | С |
| 20 | MOTA | 4433 | CB GLU L 185 | 28.562 | 95.839 | 5.023 | 1.00 82.08 | L _ | C |
| | ATOM | 4434 | CG GLU L 185 | | 95.387 | 4.788 | 1.00 82.98 | L L | C |
| | ATOM | 4435 | CD GLU L 185 | | 96.050 95.363 | 5.830 6.730 | 1.00 83.92 1.00 85.45 | L L | Ö |
| | ATOM ATOM | 4436 4437 | OE1 GLU L 185 OE2 GLU L 185 | | 97.277 | 5.847 | 1.00 83.51 | L | ŏ |
| 25 | ATOM | 4438 | C GLU L 185 | | 96.888 | 2.760 | 1.00 80.93 | L | С |
| 0 | MOTA | 4439 | O GLU L 185 | 29.750 | 97.781 | 2.573 | 1.00 79.31 | L | 0 |
| | MOTA | 4440 | N TYR L 186 | | 95.847 | 1.906 | 1.00 80.68 1.00 81.19 | L L | N C |
| | ATOM | 4441 | CA TYR L 186 CB TYR L 186 | | 95.888 94.799 | 0.600 -0.320 | 1.00 79.74 | L | Ċ |
| 30 | ATOM ATOM | 4442 4443 | CB TYR L 186 | | 94.924 | -1.735 | 1.00 79.67 | L | С |
| 50 | ATOM | 4444 | CD1 TYR L 186 | - | 95.127 | -1.986 | 1.00 79.51 | L | C |
| | ATOM | 4445 | CE1 TYR L 186 | | 94.990 | -3.274 | 1.00 78.75 | L | C |
| | ATOM | 4446 | CD2 TYR L 186 | | 94.606 | -2.809 | 1.00 79.13 1.00 78.31 | L L | C |
| 0.5 | ATOM | 4447 | CE2 TYR L 186 | | 94.472 94.669 | -4.091 -4.334 | 1.00 78.31 | L | C |
| 35 | MOTA MOTA | 4448 4449 | CZ TYR L 186 OH TYR L 186 | - | 94.670 | -5.639 | 1.00 77.89 | L | 0 |
| | ATOM | 4450 | C TYR L 186 | | 97.258 | -0.011 | 1.00 81.44 | \mathbf{L} | · C |
| | MOTA | 4451 | O TYR L 180 | | 98.023 | -0.236 | 1.00 82.62 | L | 0 |
| | MOTA | 4452 | N GLU L 18 | | 97.580 98.768 | -0.242 -0.987 | 1.00 81.21 1.00 81.63 | L L | N C |
| 40 | MOTA | 4453 4454 | CA GLU L 18' | | 98.747 | -1.066 | 1.00 82.22 | Ĺ | č |
| | ATOM ATOM | 4455 | CG GLU L 18 | | 97.889 | -2.208 | 1.00 83.98 | L | C |
| | MOTA | 4456 | CD GLU L 18 | 7 24.105 | 98.198 | -2.392 | 1.00 85.00 | L | C |
| | MOTA | 4457 | OE1 GLU L 18 | | 97.305 | -2.767 | 1.00 84.70 | L | 0 |
| 45 | ATOM | 4458 | OE2 GLU L 18' | | 99.319 100.113 | -2.073 -0.356 | 1.00 86.06 1.00 80.66 | L L | C O |
| | ATOM ATOM | 4459 4460 | O GLU L 18' | | 101.169 | -0.784 | 1.00 80.69 | L | ŏ |
| | ATOM | 4461 | N ARG L 18 | 8 28.800 | 100.085 | 0.715 | 1.00 79.90 | L | N |
| | MOTA | 4462 | CA ARG L 18 | 8 29.105 | 101.364 | 1.347 | 1.00 79.44 | Ŀ | C |
| 50 | MOTA | 4463 | CB ARG L 18 | | 101.227 | 2.864 | 1.00 80.37 1.00 82.71 | L L | C |
| | MOTA | 4464 4465 | CG ARG L 18 CD ARG L 18 | | 101.291 101.669 | 3.281 4.756 | 1.00 85.06 | L | C |
| | MOTA MOTA | 4465 | CD ARG L 18 NE ARG L 18 | | 100.484 | 5.612 | 1.00 85.93 | L | N |
| | ATOM | 4467 | CZ ARG L 18 | | 99.818 | 5.932 | 1.00 86.70 | L | C |
| 55 | MOTA | 4468 | NH1 ARG L 18 | | 100.226 | 5.477 | 1.00 86.66 | L | N |
| | ATOM | 4469 | NH2 ARG L 18 | | 98.738 101.898 | 6.716 0.973 | 1.00 86.37 1.00 78.28 | L L | N C |
| | ATOM ATOM | 4470 4471 | C ARG L 18 O ARG L 18 | | 101.090 | 1.208 | 1.00 70.20 | L | ŏ |
| | ATOM | 4472 | N HIS L 18 | | 100.835 | 0.491 | 1.00 76.81 | L | N |
| 60 | MOTA | 4473 | CA HIS L 18 | 9 32.505 | 101.005 | -0.024 | 1.00 75.77 | L | C |
| - | MOTA | 4474 | CB HIS L 18 | 9 33.450 | 100.127 | 0.793 | 1.00 76.18 | L | C |
| | MOTA | 4475 | CG HIS L 18 | | 100.344 99.803 | 2.259 3.049 | 1.00 75.83 1.00 75.79 | L L | C |
| | ATOM | 4476 4477 | CD2 HIS L 18 ND1 HIS L 18 | 34.184 3 34 056 | 101.028 | 3.049 | 1.00 76.33 | L | И |
| 65 | ATOM ATOM | 4478 | CE1 HIS L 18 | 33.568 | 100.890 | 4.306 | 1.00 76.23 | L | С |
| | ATOM | 4479 | NE2 HIS L 18 | 32.447 | 100.160 | 4.329 | 1.00 76.30 | ŗ | N |
| | ATOM | 4480 | C HIS L 18 | | 100.595 | -1.488 | 1.00 74.26 1.00 73.32 | L L | C |
| | MOTA | 4481 | O HIS L 18 | | 99.713 101.241 | -1.942 -2.203 | 1.00 73.32 | r r | N |
| | ATOM | 4482 | n asn L 19 | 0 33.495 | TAT. 747 | د.203 | 2.00 /3.22 | | -1 |

| | MOTA MOTA | 4483 4484 | CA ASN L 190 CB ASN L 190 | 33.511 33.497 | 101.062 102.448 | -3.644 -4.284 | 1.00 72.28 1.00 72.27 | L L | C |
|----|--------------|--------------|------------------------------|------------------|--------------------|------------------|--------------------------|----------------|--------|
| | ATOM | 4485 | CG ASN L 190 | 33.359 | 102.314 | -5.777 | 1.00 72.22 | Ŀ | C |
| | ATOM | 4486 | OD1 ASN L 190 | 32.582 | 101.514 | -6.291 | 1.00 72.45 | T. | 0 |
| 5 | ATOM | 4487 | ND2 ASN L 190 | 34.149 | 103.133 | -6.492 | 1.00 72.27 | L | И |
| | MOTA | 4488 | C ASN L 190 | | 100.292 | -4.083 | 1.00 71.86 1.00 71.82 | L L | C |
| | MOTA | 4489 | O ASN L 190 | 34.733 | 99.519 | -5.032 | 1.00 71.82 1.00 70.48 | F F | И |
| | ATOM | 4490 | N SER L 191 | 35.886 | | -3.430 -3.668 | 1.00 70.48 | P P | C |
| | MOTA | 4491 | CA SER L 191 | 37.231 | 99.902 100.968 | -3.415 | 1.00 68.08 | L | č |
| 10 | MOTA | 4492 | CB SER L 191 | 38.292 39.567 | | -3.635 | 1.00 70.37 | L | ŏ |
| | ATOM | .4493 | OG SER L 191 C SER L 191 | 37.561 | 98.593 | -2.756 | 1.00 68.67 | L | Č |
| | ATOM | 4494 | C SER L 191 O SER L 191 | 37.611 | 98.630 | -1.534 | 1.00 68.74 | L | 0 |
| | ATOM | 4495 4496 | N TYR L 192 | 37.721 | 97.469 | -3.426 | 1.00 67.14 | L | N |
| 15 | ATOM ATOM | 4497 | CA TYR L 192 | 37.945 | 96.133 | -2.841 | 1.00 66.18 | Ŀ | C |
| 15 | ATOM | 4498 | CB TYR L 192 | 36.809 | 95.191 | -3.337 | 1.00 64.98 | L | С |
| | ATOM | 4499 | CG TYR L 192 | 35.577 | 95.517 | -2.560 | 1.00 65.06 | L | C |
| | ATOM | 4500 | CD1 TYR L 192 | 34.690 | | -3.018 | 1.00 65.76 | Ē | C |
| | ATOM | 4501 | CE1 TYR L 192 | 33.532 | 96.850 | -2.250 | 1.00 65.52 | $ar{	t r}$ | C |
| 20 | ATOM | 4502 | CD2 TYR L 192 | 35.350 | | -1.281 | 1.00 64.44 | T. | C |
| | MOTA | 4503 | CE2 TYR L 192 | 34.192 | | -0.452 | 1.00 64.83 1.00 65.25 | L L | C |
| | MOTA | 4504 | CZ TYR L 192 | 33.299 | | -0.960 -0.300 | 1.00 65.23 | r L | Ö |
| | MOTA | 4505 | OH TYR L 192 | 32.176 39.239 | | -3.407 | 1.00 65.75 | L | č |
| | MOTA | 4506 | C TYR L 192 O TYR L 192 | 39.405 | | -4.664 | 1.00 65.70 | L | ō |
| 25 | MOTA | 4507 4508 | O TYR L 192 N THR L 193 | 40.182 | | -2.565 | 1.00 64.25 | L | N |
| | MOTA MOTA | 4509 | CA THR L 193 | 41.444 | | -2.979 | 1.00 63.31 | L | С |
| | ATOM | 4510 | CB THR L 193 | 42.465 | | -2.780 | 1.00 63.11 | ${f L}$ | С |
| | ATOM | 4511 | OG1 THR L 193 | 42.317 | | -3.840 | 1.00 63.06 | Ľ | -0 |
| 30 | ATOM | 4512 | CG2 THR L 193 | 43.903 | | -2.971 | 1.00 62.69 | Ŀ | C |
| | ATOM | 4513 | C THR L 193 | 41.943 | | -2.280 | 1.00 63.36 | L | C |
| | MOTA | 4514 | O THR L 193 | 41.741 | | -1.075 | 1.00 61.67 | L L | N O |
| | ATOM | 4515 | N CYS L 194 | 42.588 | | -3.059 | 1.00 63.76 1.00 64.62 | L | C |
| | MOTA | 4516 | CA CYS L 194 | 43.220 | | -2.686 -2.683 | 1.00 64.62 1.00 64.56 | L | Č |
| 35 | ATOM | 4517 | C CYS L 194 | 44.750 45.367 | | -3.717 | 1.00 64.27 | Ĺ | ŏ |
| | ATOM | 4518 | O CYS L 194 CB CYS L 194 | 42.754 | | -3.656 | 1.00 65.84 | L | č |
| | MOTA | 4519 4520 | CB CYS L 194 SG CYS L 194 | 43.253 | | -3.082 | 1.00 69.27 | L | S |
| | ATOM ATOM | 4521 | N GLU L 195 | 45.475 | | -1.654 | 1.00 65.49 | L | N |
| 40 | ATOM | 4522 | CA GLU L 195 | 46.940 | | -1.514 | 1.00 66.37 | L | C |
| 40 | ATOM | 4523 | CB GLU L 195 | 47.313 | | -0.485 | 1.00 67.92 | L | C |
| | ATOM | 4524 | CG GLU L 195 | 47.266 | 93.904 | -1.015 | 1.00 70.14 | Ē | C |
| | MOTA | 4525 | CD GLU L 195 | 48.023 | | -0.147 | 1.00 72.46 | Ļ | C |
| | ATOM | 4526 | OE1 GLU L 195 | 48.87 | | 0.691 | 1.00 74.03 | L L | 0 |
| 45 | MOTA | 4527 | OE2 GLU L 195 | 47.713 | | -0.294 -1.028 | 1.00 74.44 1.00 66.00 | L | C |
| | MOTA | 4528 | C GLU L 195 | 47.670 47.530 | | 0.172 | 1.00 66.57 | r. | ŏ |
| | ATOM | 4529 | O GLU L 195 | | | -1.891 | 1.00 65.28 | L | Ŋ |
| | MOTA | 4530 | N ALA L 196 CA ALA L 196 | 48.633 49.25 | | -1.699 | 1.00 64.12 | L | С |
| 50 | ATOM ATOM | 4531 4532 | CA ALA L 196 CB ALA L 196 | 49.14 | | -2.984 | 1.00 63.44 | L | C |
| 50 | ATOM | 4533 | C ALA L 196 | 50.64 | | -1.252 | 1.00 64.13 | Ŀ | С |
| | ATOM | 4534 | O ALA L 196 | 51.39 | | -1.899 | 1.00 63.42 | L | 0 |
| | MOTA | 4535 | N THR L 197 | 51.00 | | -0.064 | 1.00 64.82 | Ŀ | N |
| | ATOM | 4536 | CA THR L 197 | 52.38 | | 0.252 | 1.00 64.09 | L | C |
| 55 | MOTA | 4537 | CB THR L 197 | 52.65 | | 1.576 | 1.00 63.72 | L L | C |
| | MOTA | 4538 | OG1 THR L 197 | 52.33 | | 1.434 | 1.00 64.06 1.00 63.15 | L ₁ | Č |
| | MOTA | 4539 | CG2 THR L 197 | | | 1.879 0.070 | 1.00 64.02 | L | Č |
| | ATOM | 4540 | C THR L 197 | | | 0.788 | 1.00 64.77 | L | ŏ |
| | ATOM | 4541 | O THR L 197 N HIS L 198 | | | -0.910 | 1.00 62.84 | L | N |
| 60 | MOTA | 4542 | N HIS L 198 | | | -1.189 | 1.00 61.69 | L | С |
| | MOTA ATOM | 4543 4544 | CB HIS L 198 | | | -2.512 | 1.00 59.77 | \mathbf{L} | С |
| | ATOM | 4545 | CG HIS L 198 | | | -2.645 | 1.00 59.10 | \mathbf{r} | С |
| | ATOM | 4546 | CD2 HIS L 198 | | 2 82.226 | -2.233 | 1.00 58.46 | L | C |
| 65 | ATOM | 4547 | ND1 HIS L 198 | 55.73 | 4 83.035 | -3.297 | 1.00 59.08 | L | N |
| | ATOM | 4548 | CE1 HIS L 198 | 55.82 | | -3.331 | 1.00 57.61 | Ŀ | C |
| | MOTA | 4549 | NE2 HIS L 198 | 54.82 | | | 1.00 57.62 | L T. | N |
| | ATOM | 4550 | | | | | 1.00 61.03 1.00 60.88 | L L | C O |
| | ATOM | 4551 | O HIS L 198 | 56.74 | 7 86.720 | -1.785 | T.00 00.00 | ם | J |
| | | | | 0.4.4 | | | | | |

| 5 | ATOM 4552 N LYS L 199 ATOM 4553 CA LYS L 199 ATOM 4554 CB LYS L 199 ATOM 4555 CG LYS L 199 ATOM 4556 CD LYS L 199 ATOM 4557 CE LYS L 199 ATOM 4558 NZ LYS L 19 | 58.586 59.152 60.165 60.614 62.157 | 84.693 -1.0 84.708 -1.3 83.326 -0.0 82.579 -1.3 81.343 -0.3 81.071 -0.7 79.587 -1. | 161 1.00 6 608 1.00 6 411 1.00 6 633 1.00 6 720 1.00 6 216 1.00 7 | 1.48 2.55 5.31 7.98 88.98 72.58 | L C | |
|----|--|---|--|--|--|------------------|--|
| 10 | ATOM 4559 C LYS L 19 ATOM 4560 O LYS L 19 ATOM 4561 N THR L 20 ATOM 4562 CA THR L 20 | 59.215 60.316 58.534 58.889 | 85.037 -2. 85.439 -2. 84.770 -3. 85.151 -4. | .606 1.00 6 .867 1.00 6 .955 1.00 6 | 59.15 51.34 52.41 51.98 | L L L | C N C |
| 15 | ATOM 4563 CB THR L 20 ATOM 4564 OG1 THR L 20 ATOM 4565 CG2 THR L 20 ATOM 4566 C THR L 20 ATOM 4567 O THR L 20 | 56.492 57.965 58.937 59.287 | 84.775 -5. 83.103 -6. 86.656 -5. 87.166 -6. | .459 1.00 .030 1.00 .003 1.00 .033 1.00 .027 1.00 | 51.96 63.55 63.63 | L L L | и С С |
| 20 | ATOM 4568 N SER L 20 ATOM 4569 CA SER L 20 ATOM 4570 CB SER L 20 ATOM 4571 OG SER L 20 ATOM 4572 C SER L 20 ATOM 4573 O SER L 20 ATOM 4574 N THR L 20 | 58.503 57.270 57.317 58.532 57.824 59.389 | 88.878 -4. 89.284 -5. 90.617 -5. 89.678 -2. 89.379 -2. 90.679 -2. | .257 1.00 .062 1.00 .277 1.00 .932 1.00 .026 1.00 .903 1.00 | 66.77 66.67 69.81 67.89 | | C C C C C C C C C C |
| 25 | ATOM 4575 CA THR L 20 ATOM 4576 CB THR L 20 ATOM 4577 OG1 THR L 20 ATOM 4578 CG2 THR L 20 | 2 60.789 2 61.001 2 62.051 | 92.514 -1 92.700 -3 91.770 -1 | .942 1.00 | 70.21 71.61 69.32 71.81 | L L L | C O C C |
| 30 | ATOM 4579 C THR L 2 ATOM 4580 O THR L 2 ATOM 4581 N SER L 2 ATOM 4582 CA SER L 2 ATOM 4583 CB SER L 2 | 2 58.384 2 58.249 3 57.509 3 56.351 3 56.536 | 93.078 -0 92.620 -2 93.397 -2 94.788 -2 94.698 -4 | 1.00 2.445 1.00 2.139 1.00 2.770 1.00 4.173 1.00 | 73.06 72.08 72.51 72.61 73.89 | L L L L | О С С С С |
| 35 | ATOM 4585 C SER L 2 ATOM 4586 O SER L 2 ATOM 4587 N PRO L 2 ATOM 4588 CD PRO L 2 | 55.109 55.060 64 54.020 64 53.822 | 91.850 -3 92.809 -1 93.786 -0 | 0.890 1.00 | 73.15 73.17 73.52 73.68 73.37 | F F F | С С О |
| 40 | ATOM 4591 CG PRO L 2 ATOM 4592 C PRO L 2 ATOM 4593 O PRO L 2 | 51.760 04 52.466 04 52.319 04 52.550 | 92.891 -1 94.171 -1 92.276 -3 93.254 -4 91.345 -4 | 1.538 1.00 1.377 1.00 3.827 1.00 4.516 1.00 4.270 1.00 | 72.83 73.10 73.82 73.65 74.15 | L L L L | C C O N C |
| 45 | ATOM 4595 CA ILE L : ATOM 4596 CB ILE L : ATOM 4597 CG2 ILE L : ATOM 4598 CG1 ILE L | 05 50.947 05 51.131 05 50.847 05 50.088 | 91.530 - 90.297 - 90.291 - 90.139 - 90. | 5.470 1.00 7.496 1.00 8.411 1.00 | 75.73 77.35 75.81 76.36 | L L L | 00000 |
| 50 | ATOM 4600 C ILE L ATOM 4601 O ILE L ATOM 4602 N VAL L ATOM 4603 CA VAL L | 05 49.492 05 49.112 06 48.715 06 47.513 | 91.850 - 91.672 - 92.491 - 3 93.122 - | -4.177 1.00 -6.123 1.00 -5.663 1.00 -5.144 1.00 | 75.53 76.26 75.08 74.71 74.40 | L L L L | О И С |
| 55 | ATOM 4604 CB VAL L ATOM 4605 CG1 VAL L ATOM 4606 CG2 VAL L ATOM 4607 C VAL L ATOM 4608 O VAL L ATOM 4609 N LYS L | 206 48.952 206 47.693 206 46.644 206 47.073 | 94.812 - 9 95.650 - 4 93.211 - 1 93.738 - 2 92.674 - | -4.282 1.00 -6.301 1.00 -6.846 1.00 -7.786 1.00 -6.741 1.00 | 73.30 74.38 74.88 75.87 74.58 | L L L L | ССОИС |
| 60 | ATOM 4610 CA LYS L ATOM 4611 CB LYS L ATOM 4612 CG LYS L ATOM 4613 CD LYS L | 207 44.29 207 43.87 207 44.99 207 45.03 | 8 91.401 - 6 90.736 - 0 91.289 -1 6 90.847 -1 | -8.024 1.0 -8.978 1.0 10.379 1.0 11.268 1.0 | 0 74.35 0 74.50 0 75.19 0 76.53 0 77.77 | r r r | CCCN |
| 65 | ATOM 4614 CE LYS L ATOM 4615 NZ LYS L ATOM 4616 C LYS L ATOM 4617 O LYS L ATOM 4618 N SER L ATOM 4619 CA SER L ATOM 4620 CB SER L | 207 45.76 207 43.09 207 42.82 208 42.40 208 41.41 | 4 90.117 -1 6 93.543 7 93.341 94.355 3 95.213 | -6.906 1.0 -5.709 1.0 -7.676 1.0 -7.140 1.0 | 0 79.30 0 74.45 0 73.76 0 74.34 0 74.67 0 74.26 | L L L L | C O N C C |
| | *** *** ·· · · · · · · · · · · · · · · | 245 | | | | | |

| 5 10 15 20 25 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 4629 CI 4630 CI 4631 CI 4632 CZ 4633 C CI 4635 N 4636 CZ 4637 C CI 4638 C CI 4639 CI 4640 N 4641 C CI 4642 CI 4643 N 4644 C CI 4645 C CI 4646 C CI 4647 C CI 4648 C CI 4647 C CI 4648 C CI 4649 C CI 4649 C CI 4650 N 4651 N | SER L 208 SER L 208 PHE L 209 PHE L 210 ASN L 210 B ASN L 210 B ASN L 210 B ASN L 210 C ASN L 211 C ARG L 211 | 43.125 96.638 -6.088 1.00 75.04 L O 40.278 95.350 -8.117 1.00 75.12 L O 40.328 94.990 -9.309 1.00 75.07 L O 39.225 95.930 -7.600 1.00 75.89 L N 38.202 96.369 -8.515 1.00 76.68 L C 37.392 95.232 -8.946 1.00 75.71 L C 36.442 94.760 -7.934 1.00 76.21 L C 35.288 95.396 -7.710 1.00 76.62 L C 36.650 93.568 -7.240 1.00 76.62 L C 34.321 94.896 -6.848 1.00 76.62 L C 35.650 93.051 -6.385 1.00 77.20 L C 34.499 93.760 -6.215 1.00 77.21 L C 37.380 97.346 -7.803 1.00 78.77 |
|---------------------------|--|--|---|---|
| 35 | MOTA ATOM ATOM ATOM MOTA MOTA | 4653 C 4654 I 4655 C 4656 C 4657 C | ARG L 211 D ARG L 211 N ASN L 212 CA ASN L 212 CB ASN L 212 CG ASN L 212 | 30.298 98.696 -9.159 1.00 90.59 L O 31.609 100.529 -8.707 1.00 92.92 L N 31.022 101.615 -9.578 1.00 95.30 L C 31.287 103.060 -8.990 1.00 95.62 L C 32.727 103.685 -9.302 1.00 95.98 L C 33.706 102 985 -9.365 1.00 96.57 L O |
| 40 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 4659 1 4660 6 4661 6 4662 3 | OD1 ASN L 212 ND2 ASN L 212 C ASN L 212 O ASN L 212 N GLU L 213 CA GLU L 213 | 32.810 105.038 -9.430 1.00 95.86 L N 31.451 101.449 -11.064 1.00 97.04 L C 30.838 102.032 -11.978 1.00 97.84 L O 32.523 100.647 -11.235 1.00 98.65 L N 32.879 99.815 -12.407 1.00100.44 L C |
| 45 | MOTA MOTA MOTA MOTA MOTA | 4664 4665 4666 4667 4668 | CB GLU L 213 CG GLU L 213 CD GLU L 213 OE1 GLU L 213 OE2 GLU L 213 | 31.669 99.384 -13.335 1.00101.37 L C 30.708 98.317 -12.739 1.00103.86 L C 29.293 98.287 -13.389 1.00105.73 L C 29.148 98.663 -14.613 1.00106.92 L O 28.311 97.881 -12.696 1.00106.19 L O 34.052 100.491 -13.158 1.00101.34 L C |
| 50 | MOTA MOTA ATOM ATOM MOTA | 4670 4671 4672 4673 | C GLU L 213 O GLU L 213 OXT GLU L 213 CB ALA H 1 C ALA H 1 | 34.052 100.491 -13.136 1.00101.24 L O 35.005 101.056 -12.555 1.00101.24 L O 34.010 100.451 -14.407 1.00102.50 L O 39.945 47.058 -15.210 1.00 57.59 H C 39.240 45.311 -13.489 1.00 56.41 H C 38.014 45.283 -13.595 1.00 56.03 H O |
| 55 | MOTA MOTA MOTA MOTA MOTA | 4674 4675 4676 4677 4678 | O ALA H 1 N ALA H 1 CA ALA H 1 N VAL H 2 CA VAL H 2 | 39.647 44.577 -15.546 1.00 58.24 H N 40.167 45.578 -14.643 1.00 57.67 H C 39.812 45.198 -12.287 1.00 55.97 H N 38.982 45.072 -11.168 1.00 55.80 H C |
| 60 | MOTA MOTA MOTA MOTA | 4679 4680 4681 4682 | CB VAL H 2 CG1 VAL H 2 CG2 VAL H 2 C VAL H 2 O VAL H 2 | 38.900 44.730 -8.646 1.00 53.68 H C 40.562 43.232 -10.087 1.00 54.67 H C 38.208 46.290 -10.890 1.00 55.96 H C 38.753 47.332 -10.978 1.00 56.13 H O |
| 65 | MOTA MOTA MOTA MOTA MOTA MOTA | 4684 4685 4686 4687 4688 | N LYS H 3 CA LYS H 3 CB LYS H 3 CG LYS H 3 CD LYS H 3 CE LYS H 3 | 36.979 46.190 -10.426 1.00 55.21 H N 36.214 47.342 -10.003 1.00 54.60 H C 35.313 47.862 -11.046 1.00 56.93 H C 35.974 48.256 -12.313 1.00 61.09 H C 34.988 48.698 -13.499 1.00 64.16 H C 35.878 48.939 -14.898 1.00 66.47 H C |

| | | | | | | | | 4.5.005 | 1 00 66 | | т. | NT |
|-----|--------------|----------------|------------|--------------------|--------------|------------------|------------------|-------------------|---------------|----------------|--------|--------|
| | MOTA | | | LYS H | 3 | 35.296 35.355 | 48.156 47.206 | -16.087 -8.701 | 1.00 69 | 2.89 | H H | C N |
| | ATOM ATOM | 4691 4692 | | LYS H LYS H | 3 3 | 34.716 | 46.223 | -8.522 | 1.00 53 | | H- | 0 |
| | ATOM | 4693 | N | LEU H | 4 | 35.271 | 48.273 | -7.924 | 1.00 50 | | H H | И С |
| 5 | MOTA | 4694 | CA | LEU H | 4 | 34.437 35.301 | 48.255 48.009 | -6.746 -5.477 | 1.00 40 | | H | č |
| | ATOM ATOM | 4695 4696 | CB CG | LEU H LEU H | $rac{4}{4}$ | 36.237 | 46.878 | -5.386 | 1.00 4 | 7.93 | H | C |
| | ATOM | 4697 | CD1 | LEU H | 4 | 37.068 | 46.748 | -3.950 | 1.00 44 | 4.50 5.14 | H H | C C |
| | ATOM | 4698 | | LEU H | 4 | 35.265 | 45.686 49.504 | -5.471 -6.651 | 1.00 4 | | H | Č |
| 10 | MOTA | 4699 | C | LEU H LEU H | 4 4 | 33.768 34.443 | 50.510 | -6.706 | 1.00 4 | 9.93 | H | 0 |
| | ATOM ATOM | $4700 \\ 4701$ | N O | VAL H | 5 | 32.466 | 49.494 | -6.457 | | 8.58 | H | N |
| | ATOM | 4702 | CA | VAL H | 5 | 31.680 | 50.754 | -6.411 | 1.004 1.004 | 8.51 8.35 | H H | C C |
| | MOTA | 4703 | CB | VAL H | 5 | 30.892 30.080 | 50.955 52.257 | -7.693 -7.619 | 1.00 4 | 7.31 | H | Č |
| 15 | MOTA | 4704 4705 | | VAL H | 5 5 | 31.859 | 50.919 | -8.930 | 1.00 4 | 6.39 | H | C |
| | MOTA MOTA | 4705 4706 | C | VAL H | 5 | 30.742 | 50.824 | -5.191 | 1.00 4 | | H H | C O |
| | MOTA | 4707 | 0 | VAL H | 5 | 29.722 | 50.175 51.695 | -5.154 -4.269 | 1.004 1.004 | 9.40 | Н | N |
| | ATOM | 4708 | N | GLU H | 6 6 | 31.058 30.241 | 51.844 | -3.056 | 1.00 5 | | H | C |
| 20 | MOTA ATOM | 4709 4710 | CA CB | GLU H | 6 | 31.120 | 52.542 | -2.043 | | 0.52 | H | C |
| | ATOM | 4711 | CG | GLU H | 6 | 32.410 | 51.720 | -1.614 -2.427 | | 2.97 4.93 | H H | C C |
| | MOTA | 4712 | CD | GLU H | 6 | 33.634 33.454 | 52.070 52.594 | -2.427 -3.591 | 1.00 5 | | H | ŏ |
| 0.5 | MOTA | 4713 4714 | OE1 OE2 | | 6 6 | 34.778 | 51.772 | -1.950 | 1.00 5 | 3.24 | H | 0 |
| 25 | MOTA MOTA | 4715 | C | GLU H | 6 | 29.005 | 52.674 | -3.334 | | 1.92 | H H | C O |
| | MOTA | 4716 | 0 | GLU H | 6 | 29.006 | 53.587 52.409 | -4.190 -2.617 | | 3.20 52.28 | H | И |
| | MOTA | 4717 | N | SER H SER H | 7 7 | 27.949 26.784 | 53.228 | -2.628 | 1.00 5 | | H | С |
| 30 | ATOM ATOM | 4718 4719 | CA CB | SER H | 7 | 25.870 | 52.850 | -3.832 | | 51.14 | H | C |
| 30 | ATOM | 4720 | ŌĠ | SER H | 7 | 25.351 | 51.648 | | 1.00 5 | | H H | 0 |
| | MOTA | 4721 | C | SER H | 7 | 26.041 26.407 | 53.138 52.356 | | 1.00 5 | 52.35 | Н | ō |
| | MOTA | 4722 4723 | N O | SER H GLY H | 7 8 | 24.926 | 53.908 | | 1.00 5 | 53.91 | Н | N |
| 35 | ATOM ATOM | 4724 | CA | GLY H | 8 | 24.156 | 53.922 | | 1.00 5 | | H H | C C |
| - | ATOM | 4725 | C | GLY H | 8 | 24.571 23.988 | 54.962 55.136 | | 1.00 | | H | Ö |
| | ATOM | 4726 | O | GLY H | 8 9 | 25.549 | 55.685 | | | 54.06 | H | N |
| | ATOM ATOM | 4727 4728 | N CA | GLY H | 9 | 26.023 | 56.605 | 1.797 | | 55.85 | H H | C |
| 40 | ATOM | 4729 | C | GLY H | 9 | 25.094 | 57.863 | | | 56.97 58.21 | H | Ö |
| | ATOM | 4730 | 0 | GLY H | 9 10 | 24.395 25.096 | 58.190 58.589 | | | 56.93 | H | N |
| | MOTA MOTA | 4731 4732 | N CA | | 10 | 24.492 | 59.891 | L 3.099 | 1.00 | | H | C |
| | MOTA | 4733 | C | GLY H | 10 | 24.458 | 60.322 | | | 57.22 56.37 | H H | C |
| 45 | MOTA | 4734 | 0 | GLY H | 10 | 25.269 23.491 | 59.948 61.158 | | | | H | N |
| | MOTA | 4735 4736 | N CA | LEU H | 11 11 | 23.324 | | - | 1.00 | 58.33 | H | C |
| | MOTA MOTA | 4737 | CB | | 11 | 22.670 | 63.09 | 5.971 | | 57.28 | H H | C C |
| | ATOM | 4738 | CG | LEU H | 11 | 22.217 23.399 | | | | 57.41 56.59 | H | С |
| 50 | ATOM | 4739 | | 1 LEU H 2 LEU H | 11 11 | 23.533 | | | 1.00 | 55.33 | H | С |
| | ATOM ATOM | 4740 4741 | | LEU H | 11 | 22.422 | 60.91 | 2 7.021 | | 58.53 | H H | C O |
| | ATOM | 4742 | | LEU H | 11 | 21.366 | | | | 59.22 58.84 | H | N |
| | ATOM | 4743 | | VAL H | 12 12 | 22.718 21.708 | | | | 59.95 | H | С |
| 55 | MOTA ATOM | 4744 4745 | | | 12 | 22.077 | | 7 8.929 | 1.00 | 60.75 | H | C |
| | ATOM | 4746 | CG | 31 VAL H | 12 | 23.568 | | | | 60.56 60.62 | H H | C |
| | ATOM | 4747 | | 2 VAL H | 12 | 21.161 21.774 | | | | 60.49 | H | č |
| | MOTA | 4748 | | VAL H VAL H | 12 12 | 22.697 | | | 9 1.00 | 60.65 | H | 0 |
| 60 | MOTA MOTA | 4749 4750 | | LYS H | | 20.834 | 60.19 | 5 11.25 | | 60.42 | H | N C |
| | MOTA | 4751 | L CF | A LYS H | 13 | 20.867 | | | | 59.46 60.98 | H H | C |
| | MOTA | 4752 | | | | 19.419 18.779 | | | 1 1.00 | 63.17 | H | С |
| e e | MOTA MOTA | 4753 4754 | | | _ | 17.763 | | 4 13.15 | 4 1.00 | 65.62 | H | C |
| 65 | MOTA | | | | 13 | 17.036 | 64.15 | 4 12.22 | | 68.26 71.07 | H H | и С |
| | ATOM | 4756 | S N | | | 16.293 21.483 | | | | 58.33 | H | Č |
| | MOTA | | | | | 21.48 | | | | 58.31 | H | 0 |
| | ATOM | 4758 | . 0 | יו מיות | | 247 | | | | | | |

| | ATOM ATOM ATOM ATOM | 4760 4761 | | PRO H PRO H PRO H PRO H | 14 14 14 14 | 22.042 22.318 22.626 22.995 | 60.411 61.869 59.548 60.555 | 14.752 14.891 15.802 16.947 | 1.00 57.07 1.00 55.75 1.00 56.28 1.00 56.53 | н н н | N C C |
|----|--|--|------------------------------|---|--------------------------------------|--|---|--|--|----------------------------|---------------------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM | | CG C O N CA | PRO H PRO H PRO H GLY H GLY H | 14 14 14 15 15 | 23.122 21.666 20.570 21.993 20.994 | 61.877 58.517 58.933 57.257 56.241 | 16.191 16.305 16.728 16.354 16.724 | 1.00 56.41 1.00 55.92 1.00 56.88 1.00 55.44 1.00 54.88 | н н н н | С С С |
| 10 | ATOM ATOM ATOM ATOM | 4768 4769 4770 4771 | C O N CA | GLY H GLY H GLY H GLY H | 15 15 16 16 16 | 20.484 19.892 20.699 19.951 20.773 | 55.495 54.476 56.038 55.543 54.494 | 15.465 15.544 14.263 13.101 12.482 | 1.00 54.20 1.00 54.74 1.00 53.14 1.00 51.86 1.00 52.00 | н н н н | |
| 15 | ATOM ATOM ATOM ATOM ATOM | 4772 4773 4774 4775 4776 | C N CA CB | GLY H SER H SER H SER H | 16 17 17 17 | 21.729 20.297 20.774 19.762 20.092 | 53.970 54.042 52.845 51.729 51.111 | 13.145 11.307 10.687 10.752 12.020 | 1.00 51.59 1.00 53.11 1.00 54.45 1.00 54.70 1.00 59.63 | н н н н | N C C |
| 20 | ATOM ATOM ATOM ATOM ATOM | 4777 4778 4779 4780 4781 | OG C O N CA | SER H SER H SER H LEU H LEU H | 17 17 17 18 18 | 20.920 20.163 21.938 22.072 | 53.091 53.853 52.505 52.699 | 9.213 8.685 8.621 7.169 6.955 | 1.00 54.40 1.00 53.44 1.00 54.00 1.00 54.73 1.00 54.70 | H H H H | C O N C |
| 25 | ATOM ATOM ATOM ATOM ATOM | 4782 4783 4784 4785 4786 | | LEU H LEU H LEU H | 18 18 18 18 | 22.948 23.142 21.896 24.212 22.774 | 54.458 55.216 55.423 51.412 | 5.572 5.078 5.601 6.623 | 1.00 56.43 1.00 56.27 1.00 56.44 1.00 55.38 | H H H H | |
| 30 | ATOM ATOM ATOM ATOM ATOM | 4787 4788 4789 4790 4791 | O N CA CB CG | LEU H LYS H LYS H LYS H LYS H | 18 19 19 19 19 | 23.624 22.509 23.140 22.060 22.453 | 51.140 50.022 48.990 | 7.374 5.353 4.821 4.581 3.743 | 1.00 56.00 1.00 53.52 1.00 53.55 1.00 56.27 1.00 58.99 | H H H | I N I C I C |
| 35 | MOTA MOTA MOTA | 4792 4793 4794 4795 | CD CE NZ C | LYS H LYS H LYS H LYS H LYS H | 19 19 19 19 | 21.232 21.663 20.773 23.873 23.232 | 3 45.114 L 44.171 L 50.392 | | 1.00 61.93 1.00 63.64 1.00 65.48 1.00 52.35 1.00 50.72 | 1- 1- 1- 1- 1- | H C |
| 40 | MOTA MOTA MOTA MOTA MOTA | 4796 4797 4798 4799 4800 | O N CA CB CG | LEU H LEU H LEU H | 20 20 20 20 | 25.196 25.95 27.363 27.433 | 50.059 7 50.334 1 50.733 9 51.809 | 3.504 2.258 2.749 3.840 | 1.00 50.39 1.00 49.11 1.00 47.89 1.00 47.60 1.00 43.14 | | ı C |
| 45 | MOTA MOTA MOTA MOTA MOTA | 4801 4802 4803 4804 4805 | | LEU H LEU H LEU H LEU H SER H | 20 20 20 20 21 | 28.975 26.685 26.055 25.99 26.44 | 2 53.096 8 49.092 9 47.926 6 49.281 | 3.407 1.342 1.817 0.097 | 1.00 43.08 1.00 48.76 1.00 48.50 1.00 47.53 | I I I | H C H C H O |
| 50 | ATOM ATOM ATOM ATOM | 4806 4807 4808 4809 4810 | CA CB OG C | SER H SER H SER H SER H | 21 21 21 | 26.57 25.23 24.93 27.72 28.30 | 0 47.952 1 48.983 7 48.498 | -1.286 -2.110 -1.651 | 1.00 53.28 1.00 50.26 |]]] | H C H C H C H C |
| 55 | ATOM ATOM ATOM ATOM ATOM ATOM | 4811 4812 4813 4814 4815 | O N CA C O CB | CYS H CYS H CYS H CYS H | 22 22 22 22 22 22 | 28.24 29.41 29.34 29.35 30.76 32.24 | 4 47.418 2 47.531 6 46.503 7 45.322 1 47.352 | -2.228 -3.065 -4.180 -3.900 -2.238 | 1.00 50.61 1.00 50.77 1.00 50.55 1.00 50.98 1.00 51.71 | | H CH CH CH CH CH S |
| 60 | ATOM ATOM ATOM ATOM ATOM | 4816 4817 4818 4819 4820 | SG N CA CB | CYS H ALA H ALA H ALA H | 23 23 23 23 23 | 29.41 29.30 28.61 30.60 31.27 | 5 46.993 2 46.234 4 47.108 4 45.935 | 3 -5.373 4 -6.577 3 -7.567 5 -7.103 | 1.00 49.89 1.00 49.03 1.00 47.99 1.00 49.69 | | H N H C H C H C |
| 65 | MOTA MOTA MOTA MOTA MOTA | 4821 4822 4823 4824 4825 4826 | O N CA CB C | ALA H ALA H ALA H | I 24 I 24 I 24 I 24 I 24 | 30.91 32.20 32.73 32.14 31.35 | 1 44.676 17 44.285 1 43.146 13 43.718 14 42.919 | 6 -7.200 5 -7.697 0 -6.924 8 -9.135 9 -9.301 | 1.00 49.14 1.00 48.47 1.00 47.00 1.00 48.34 1.00 49.22 | | H N H C H C H O H N |
| | MOTA | 4827 | N | SER F | 1 25 | 33.30 | 14 43.10 | O -2.010 | , 1.00 40.04 | | |

| | ATOM ATOM | 4828 4829 | | ER H | 25 25 | 33.438 32.645 | 43.147 · 44.055 · | -12.109 | 1.00 45.88 1.00 45.88 | H H | C |
|-----|--------------|--------------|---------|----------------|----------|------------------|-------------------|-----------------------|--------------------------|--------|--------|
| | MOTA | 4830 | | ER H | 25 | 33.287 | 45.345 | | 1.00 45.34 1.00 45.41 | H H | 0 |
| _ | MOTA | 4831 | | ER H | 25 | 34.889 | 43.038 43.637 | -11.463 | 1.00 43.41 | · H | C O |
| 5 | MOTA | 4832 | | ER H | 25 | 35.874 35.133 | | -10.833 | 1.00 45.42 | H | И |
| | MOTA | 4833 4834 | | TA H TA H | 26 26 | 36.533 | 42.204 | | 1.00 44.78 | H | Ĉ |
| | ATOM ATOM | 4835 | | TA H | 26 | 37.332 | | -12.147 | 1.00 45.64 | H | č |
| | ATOM | 4836 | | LY H | 26 | 38.405 | 40.867 | | 1.00 47.57 | H | 0 |
| 10 | ATOM | 4837 | | HE H | 27 | 36.715 | 40.205 | | 1.00 45.58 | H | N |
| | ATOM | 4838 | CA F | HE H | 27 | 37.357 | | -10.671 | 1.00 46.08 | H | C |
| | MOTA | 4839 | CB F | PHE H | 27 | 38.317 | 39.699 | -9.644 | 1.00 43.87 | H | C |
| | MOTA | 4840 | | HE H | 27 | 37.579 | 40.292 | -8.414 | 1.00 43.88 | H | C C |
| | ATOM . | 4841 | | PHE H | 27 | 37.326 | 39.512 | -7.245 -8.474 | 1.00 40.50 1.00 42.67 | H H | C |
| 15 | ATOM | 4842 | | PHE H | 27 27 | 37.119 36.667 | 41.532 40.059 | -6.196 | 1.00 42.07 | H | č |
| | ATOM ATOM | 4843 4844 | | PHE H | 27 | 36.366 | 42.142 | -7.299 | 1.00 44.46 | H | č |
| | ATOM | 4845 | | PHE H | 27 | 36.134 | 41.425 | -6.272 | 1.00 42.65 | H | C |
| | ATOM | 4846 | | PHE H | 27 | 36.336 | | -10.076 | 1.00 47.08 | H | C |
| 20 | ATOM | 4847 | - | PHE H | 27 | 35.185 | 38.307 | -9.844 | 1.00 49.16 | H | 0 |
| | MOTA | 4848 | N J | CHR H | 28 | 36.748 | 36.820 | -9.877 | 1.00 48.35 | H | N |
| | ATOM | 4849 | | CHR H | 28 | 35.813 | 35.893 | -9.410 | 1.00 50.12 | H H | C |
| | ATOM | 4850 | | THR H | 28 | 36.202 | 34.434 | -9.933 -9.243 | 1.00 52.14 1.00 56.55 | н Н | o |
| 0.5 | MOTA | 4851 | | PHR H PHR H | 28 28 | 35.403 37.402 | 33.362 34.188 | -9.243 -9.641 | 1.00 53.83 | H | Č |
| 25 | MOTA MOTA | 4852 4853 | | THR H | 28 | 35.514 | 36.102 | -7.818 | 1.00 49.21 | H | Č |
| | ATOM | 4854 | | THR H | 28 | 36.115 | 35.568 | -6.977 | 1.00 49.79 | H | 0 |
| | ATOM | 4855 | | PHE H | 29 | 34.524 | 36.874 | -7.593 | 1.00 47.72 | H | N |
| | ATOM | 4856 | | PHE H | 29 | 34.149 | 37.342 | -6.286 | 1.00 47.97 | H | |
| 30 | ATOM | 4857 | | PHE H | 29 | 32.787 | 38.132 | -6.445 | 1.00 47.14 | H | C |
| | MOTA | 4858 | | PHE H | 29 | 32.172 | 38.691 | -5.220 | 1.00 49.20 1.00 48.92 | H H | |
| | ATOM | 4859 | | PHE H | 29 | 32.709 | 39.718 38.144 | -4.625 -4.646 | 1.00 48.92 | H | |
| | MOTA | 4860. | | PHE H PHE H | 29 29 | 31.027 32.193 | 40.292 | -3.574 | 1.00 30.52 | H | |
| 35 | ATOM ATOM | 4861 4862 | | PHE H | 29 | 30.519 | 38.683 | -3.472 | 1.00 51.60 | H | |
| 35 | ATOM | 4863 | | PHE H | 29 | 31.069 | 39.875 | -3.036 | 1.00 50.36 | H | |
| | MOTA | 4864 | | PHE H | 29 | 34.066 | 36.255 | -5.324 | 1.00 48.25 | H | |
| | ATOM | 4865 | | PHE H | 29 | 34.650 | 36.405 | -4.308 | 1.00 47.87 | H | |
| | ATOM | 4866 | | ILE H | 30 | 33.416 | 35.161 | -5.640 | 1.00 48.05 | H | |
| 40 | ATOM | 4867 | _ | ILE H | 30 | 33.240 | 34.134 | -4.657 | 1.00 48.95 1.00 51.25 | H H | |
| | ATOM | 4868 | | ILE H | 30 30 | 32.439 31.085 | 32.942 33.450 | -5.181 -5.918 | 1.00 51.25 | Н | |
| | ATOM ATOM | 4869 4870 | | ILE H | 30 | 33.251 | 32.358 | -6.337 | 1.00 53.67 | H | |
| | ATOM | 4871 | | ILE H | 30 | 32.533 | 31.000 | -6.629 | 1.00 56.77 | H | |
| 45 | ATOM | 4872 | | ILE H | 30 | 34.510 | 33.607 | -4.067 | 1.00 47.10 | H | |
| | ATOM | 4873 | | ILE H | 30 | 34.426 | 33.078 | -2.972 | 1.00 46.72 | H | |
| | MOTA | 4874 | | SER H | 31 | 35.639 | 33.649 | -4.781 | 1.00 45.74 | H | |
| | MOTA | 4875 | | SER H | 31 | 36.879 | 33.125 | -4.259 | 1.00 46.34 1.00 45.27 | H H | |
| 50 | ATOM | 4876 | | SER H | 31 31 | 37.827 37.519 | 32.857 31.569 | -5.438 -6.102 | 1.00 47.34 | H | |
| 50 | MOTA MOTA | 4877 4878 | | SER H | 31 | 37.608 | 34.041 | -3.249 | 1.00 47.42 | H | |
| | ATOM | 4879 | | SER H | 31 | 38.528 | 33.582 | -2.645 | 1.00 48.51 | Н | |
| | ATOM | 4880 | | TYR H | 32 | 37.258 | 35.349 | -3.166 | 1.00 46.52 | H | |
| | MOTA | 4881 | | TYR H | 32 | 37.975 | 36.322 | -2.352 | 1.00 45.49 | H | |
| 55 | MOTA | 4882 | | TYR H | 32 | 38.213 | 37.568 | -3.172 | 1.00 45.29 | H | |
| | MOTA | 4883 | | TYR H | 32 | 39.251 | 37.376 | -4.152 | 1.00 47.58 1.00 46.72 | H H | |
| | MOTA | 4884 | | TYR H | 32 | 38.922 | 36.939 36.713 | -5.514 -6.359 | 1.00 47.22 | H | |
| | MOTA | 4885 | _ | TYR H | 32 32 | 39.847 40.590 | 37.593 | -3.856 | 1.00 47.39 | H | |
| 60 | ATOM ATOM | 4886 4887 | | TYR H | 32 | 41.530 | 37.455 | -4.906 | 1.00 49.71 | H | I C |
| 00 | ATOM | 4888 | | TYR H | 32 | 41.051 | 36.937 | -6.187 | 1.00 49.39 | H | ı C |
| | ATOM | 4889 | | TYR H | 32 | 41.962 | 36.800 | -7.206 | 1.00 50.64 | H | 0 1 |
| | ATOM | 4890 | C | TYR H | 32 | 37.216 | 36.750 | -1.113 | 1.00 44.53 | H | |
| | ATOM | 4891 | | TYR H | 32 | 35.949 | 36.960 | -1.073 | 1.00 43.26 | H | |
| 65 | MOTA | 4892 | | ALA H | 33 | 37.935 | 36.900 | -0.101 | 1.00 42.87 1.00 42.63 | H H | |
| | ATOM | 4893 | | ALA H | 33 | 37.400 | 37.574 37.424 | $\frac{1.210}{2.247}$ | 1.00 42.03 | H | |
| | ATOM | 4894 4895 | CB C | ALA H | 33 33 | 38.336 37.328 | 39.121 | 0.848 | 1.00 41.98 | H | |
| | MOTA MOTA | 4896 | O | ALA H | 33 | 38.029 | 39.563 | -0.026 | 1.00 41.34 | H | |
| | | | | | | | | | | | |

| | - | 36 474 39.866 1.481 1.00 41.20 | H N |
|----|--|--|------------|
| | ATOM 4897 N MET H 34 ATOM 4898 CA MET H 34 | 36.186 41.225 1.222 1.00 40.63 36.186 41.225 1.222 1.00 39 10 | H C H C |
| | ATOM 4899 CB MET H 34 | 34.605 40.629 -0.882 1.00 39.77 | H C |
| 5 | ATOM 4901 SD MET H 34 | 35.784 41.463 -1.994 1.00 45.71 34.886 42.882 -1.964 1.00 37.92 | н С |
| | ATOM 4902 CE MET H 34 ATOM 4903 C MET H 34 | 36.064 41.971 2.628 1.00 41.20 | H C H O |
| | ATOM 4904 O MET H 34 | 36 215 43.285 2.610 1.00 41.11 | H N |
| 10 | ATOM 4906 CA SER H 35 | 36.200 44.080 3.829 1.00 42.00 | H C H C |
| 10 | ATOM 4907 CB SER H 35 | 38.364 43.036 4.454 1.00 47.79 | H О H С |
| | ATOM 4909 C SER H 35 | 35.695 45.455 3.673 1.00 41.71 35.720 46.062 2.568 1.00 41.47 | н О |
| 15 | ATOM 4910 O SER H 35 ATOM 4911 N TRP H 36 | 35.278 46.065 4.802 1.00 42.04 | H N H C |
| 15 | ATOM 4912 CA TRP H 36 | 33.732 47.837 5.384 1.00 40.20 | H C |
| | ATOM 4914 CG TRP H 36 | 32.757 47.463 4.576 1.00 43.62 | н С |
| | ATOM 4915 CD2 TRP H 36 | 31.210 47.285 2.887 1.00 45.57 | н С н С |
| 20 | ATOM 4917 CE3 TRP H 36 | 32 184 46.211 4.564 1.00 44.58 | н С |
| | ATOM 4919 NE1 TRP H 36 | 31.199 46.152 3.621 1.00 44.93 | H N H C |
| | ATOM 4920 CZ2 TRP H 36 | 31.538 49.746 1.866 1.00 47.87 | н С н С |
| 25 | ATOM 4922 CH2 TRP H 36 | 30.542 48.889 1.300 1.00 47.68 36.263 48.226 5.552 1.00 41.16 | н С |
| | ATOM 4923 C TRP H 36 ATOM 4924 O TRP H 36 | 36.743 47.750 6.656 1.00 41.65 | H O |
| | ATOM 4925 N VAL H 37 | 37.677 50.161 5.817 1.00 41.72 | н С н С |
| 30 | ATOM 4927 CB VAL H 37 | 39.036 50.109 5.144 1.00 42.37 40.071 51.091 5.876 1.00 39.85 | н С |
| | ATOM 4928 CG1 VAL H 37 ATOM 4929 CG2 VAL H 37 | 39.663 48.676 5.106 1.00 38.47 | н С н С |
| | ATOM 4930 C VAL H 37 | 36 995 52.089 4.630 1.00 42.66 | н О |
| 35 | ATOM 4932 N ARG H 38 | 37.228 52.304 6.833 1.00 44.32 | н N н С |
| | ATOM 4933 CA ARG H 38 | 35.669 53.856 7.939 1.00 45.50 | н С н С |
| | ATOM 4935 CG ARG H 38 | 36.084 53.725 9.186 1.00 45.79 34.803 53.785 10.025 1.00 45.99 | H C |
| 40 | ATOM 4936 CD ARG H 38 ATOM 4937 NE ARG H 38 | 35.170 53.623 11.372 1.00 45.09 | H N H C |
| | ATOM 4938 CZ ARG H 38 | 32.926 53.654 12.247 1.00 45.96 | H N H N |
| | ATOM 4940 NH2 ARG H 38 | 34.638 53.487 13.675 1.00 45.71 | н С |
| 45 | ATOM 4941 C ARG H 38 ATOM 4942 O ARG H 38 | 38.903 54.408 7.622 1.00 45.24 | H O H N |
| | ATOM 4943 N GLN H 39 | 38.673 56.948 6.926 1.00 47.06 | H C |
| | ATOM 4945 CB GLN H 39 | 39.308 57.430 5.570 1.00 46.43 | н С |
| 50 | ATOM 4946 CG GLN H 39 | 41.330 58.532 4.518 1.00 47.35 | н С н О |
| | ATOM 4948 OE1 GLN H 39 | 40.833 50.575 4.792 1.00 45.77 | H N |
| | ATOM 4950 C GLN H 39 | 37.956 58.115 7.601 1.00 47.56 | н С н О |
| 55 | ATOM 4951 O GLN H 39 | 38.514 58.593 8.660 1.00 48.24 | H N H C |
| | ATOM 4953 CA THR H 40 | 37.841 59.686 9.468 1.00 50.75 | н С |
| | ATOM 4954 CB THR H 40 ATOM 4955 OG1 THR H 40 | 39.707 60.030 10.772 1.00 52.70 | н О н С |
| 60 | ATOM 4956 CG2 THR H 40 | 30 346 60 985 8.902 1.00 51.36 | н С |
| | ATOM 4957 C THR H 40 ATOM 4958 O THR H 40 | 39.059 61.013 8.038 1.00 51.10 | O H |
| | ATOM 4959 N PRO H 41 | 36.295 62.115 10.073 1.00 52.24 | н с |
| 65 | ATOM 4961 CA PRO H 41 | 37.890 63.382 8.700 1.00 51.01 | н С |
| 00 | ATOM 4962 CB PRO H 41 | 35.639 63.438 9.554 1.00 50.96 | н С н С |
| | ATOM 4964 C PRO H 41 | 39.303 63.781 9.025 1.00 51.27 39.846 64.518 8.265 1.00 51.34 | н О |
| | ATOM 4965 O PRO H 41 | 250 | |

| 5 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 4966 4967 4968 4969 4970 4971 4972 | CA CB CCC CCC CCCCCCCCCCCCCCCCCCCCCCCCC | GLU H GLU H GLU H GLU H GLU H | 42 42 42 42 42 42 42 | 39.838 41.210 41.532 40.596 39.079 38.707 38.252 | 63.399 63.665 63.339 64.039 63.416 62.251 63.979 | 10.184 10.527 12.031 13.179 13.163 13.758 12.323 | 1.00 50.91 1.00 52.30 1.00 55.58 1.00 59.66 1.00 62.60 1.00 63.38 1.00 64.12 | н н н н н | иссссоо |
|----|--|--|---|---|--|--|--|--|--|----------------------------|------------------|
| 10 | ATOM ATOM ATOM ATOM ATOM ATOM | 4973 4974 4975 4976 4977 4978 | C C C C C C | GLU H GLU H ALA H ALA H ALA H ALA H | 42 42 43 43 43 | 42.073 43.240 41.527 42.347 43.348 43.018 43.689 | 62.709 62.735 61.853 61.082 61.928 59.830 59.136 | 9.628 9.742 8.757 7.706 6.815 8.352 7.699 | 1.00 51.81 1.00 52.65 1.00 49.44 1.00 48.63 1.00 47.37 1.00 48.33 1.00 48.60 | H H H H H H | 000000 |
| 15 | ATOM ATOM ATOM ATOM ATOM | 4979 4980 4981 4982 4983 | N CA CB CG | ALA H ARG H ARG H ARG H ARG H | 43 44 44 44 | 42.570 42.889 42.938 44.321 | 59.389 58.032 57.885 58.813 | 9.572 9.839 11.296 11.780 | 1.00 47.49 1.00 48.90 1.00 52.09 1.00 59.28 | н н н н | С С С |
| 20 | MOTA MOTA MOTA | 4984 4985 4986 4987 4988 | NE CZ NH1 | ARG H ARG H ARG H ARG H | 44 44 44 44 | 44.773 45.692 46.987 47.689 47.593 | 58.725 57.571 57.605 58.789 56.430 | 13.290 13.544 13.921 14.061 14.154 | 1.00 62.11 1.00 64.30 1.00 63.28 1.00 63.13 1.00 63.84 | н н н н | N C N |
| 25 | ATOM ATOM ATOM ATOM ATOM | 4989 4990 4991 4992 | C O N CA | ARG H ARG H LEU H LEU H | 44 44 45 45 | 42.073 40.898 42.750 42.201 | 56.938 56.964 55.849 54.621 | 9.226 9.436 8.788 8.474 7.427 | 1.00 47.27 1.00 47.74 1.00 44.62 1.00 43.21 1.00 41.37 | н н н н | С О И С |
| 30 | ATOM ATOM ATOM ATOM ATOM | 4993 4994 4995 4996 4997 | | LEU H LEU H LEU H LEU H | 45 45 45 45 45 | 42.979 43.190 44.344 42.020 41.890 | 53.927 54.958 54.453 54.769 53.725 | 6.126 5.241 5.365 9.680 | 1.00 41.08 1.00 39.01 1.00 41.28 1.00 44.41 | Н Н Н Н | C C C |
| 35 | ATOM ATOM ATOM ATOM ATOM | 4998 4999 5000 5001 5002 | O N CA CB CG | LEU H GLU H GLU H GLU H | 45 46 46 46 46 | 42.784 40.653 40.405 39.654 38.953 37.945 | 53.297 53.243 52.104 52.733 51.754 52.324 | 10.506 9.616 10.572 11.793 12.667 13.608 | 1.00 42.31 1.00 44.35 1.00 46.78 1.00 48.43 1.00 52.62 1.00 56.08 | Н Н Н Н Н | 0 12 0 0 0 |
| 40 | MOTA TOM ATOM ATOM ATOM ATOM | 5003 5004 5005 5006 5007 | CD OE1 OE2 C | | 46 46 46 46 | 37.478 37.788 39.651 38.667 40.175 | 53.515 51.555 50.915 51.058 49.729 | 13.325 14.649 9.850 9.176 9.965 | 1.00 57.26 1.00 55.19 1.00 46.71 1.00 46.44 1.00 46.18 | Н Н Н Н | и С О |
| 45 | ATOM ATOM ATOM ATOM ATOM | 5008 5009 5010 5011 5012 | N CA CB CG CD2 | TRP H TRP H TRP H | 47 47 47 47 | 39.466 40.340 39.694 39.356 38.668 | 48.450 47.263 45.993 45.041 44.028 | 9.572 9.895 9.682 10.644 | 1.00 46.26 1.00 45.60 1.00 49.04 1.00 49.15 1.00 48.82 | Н Н Н Н | 00000 |
| 50 | ATOM ATOM ATOM ATOM ATOM | 5013 5014 5015 5016 5017 | NE1 CZ2 | TRP H TRP H TRP H TRP H | 1 47 1 47 1 47 1 47 | 39.556 39.199 38.624 38.166 39.025 | 44.952 45.536 44.341 42.946 43.894 | 12.113 8.452 8.636 10.626 | 1.00 49.50 1.00 47.78 1.00 48.17 1.00 49.29 | H H H H | С И С |
| 55 | ATOM ATOM ATOM ATOM ATOM | 5018 5019 5020 5021 5022 | О С | TRP F TRP F TRP F VAL F | 1 47 1 47 1 47 1 48 | 38.534 38.178 38.089 37.138 | 42.753 48.290 48.496 48.043 | 11.972 10.228 11.428 9.468 | 1.00 49.96 1.00 45.51 1.00 46.18 1.00 45.21 | Н Н Н Н | Д С С |
| 60 | ATOM ATOM ATOM ATOM ATOM | 5023 5024 5025 5026 5027 | CB CG1 CG2 | VAL I VAL I VAL I VAL I VAL I | 4 48 4 48 4 48 | 35.778 34.909 33.524 35.317 35.150 | 49.056 48.931 50.434 46.594 | 9.097 9.243 9.519 9.919 | 1.00 46.39 1.00 46.00 1.00 46.55 1.00 47.74 | Н Н Н Н | 2000 |
| 65 | ATOM ATOM ATOM ATOM ATOM ATOM | 5028 5029 5030 5031 5032 5033 | O N CA CB C | VAL I ALA I ALA I ALA I ALA I | H 48 H 49 H 49 H 49 H 49 H 49 | 34.364 35.430 34.934 33.393 35.447 35.923 | 45.788 44.439 44.443 43.653 44.124 | 8.912 9.013 9.047 3.7.835 4.6.750 | 1.00 47.88 1.00 47.12 1.00 47.13 1.00 46.52 1.00 46.49 | н н н н н | и оооо ои |
| | MOTA | 5034 | ł N | SER ! | H 50 | 33.410 | , -12.57. | _ 0.0,2 | | | |

| | ATOM | | CA SER H | 50 | 35.824 | 41.422 | 6.964 7.351 | 1.00 45.97 1.00 45.68 | H H | C |
|----|--------------|--------------|---------------------|----------|------------------|--------------------|------------------|--------------------------|--------|--------|
| | MOTA | | CB SER H | 50 50 | 37.267 38.110 | 40.907 41.991 | 7.172 | 1.00 46.90 | H | ŏ |
| | MOTA | | OG SER H C SER H | 50 50 | 34.842 | 40.237 | 6.905 | 1.00 45.95 | H | C |
| - | MOTA MOTA | | C SER H O SER H | | 34.224 | 39.839 | 7.964 | 1.00 46.23 | H | 0 |
| 5 | ATOM | | N ILE H | 51 | 34.740 | 39.574 | 5.746 | 1.00 44.35 | H | N |
| | ATOM | | CA ILE H | | 34.061 | 38.321 | 5.575 | 1.00 43.41 | H | C C |
| | ATOM | | CB ILE H | | 32.647 | 38.545 | 4.897 | 1.00 42.37 1.00 40.16 | H H | C |
| | MOTA | | CG2 ILE H | | 32.703 | 39.310 37.239 | 3.471 4.824 | 1.00 41.84 | H | č |
| 10 | ATOM | | CG1 ILE H | | 31.811 30.240 | 37.456 | 4.666 | 1.00 41.59 | H | С |
| | MOTA | | CD1 ILE H | | 34.881 | 37.441 | 4.640 | 1.00 44.63 | H | C |
| | MOTA MOTA | | O ILE H | | 35.403 | 38.002 | 3.596 | 1.00 44.42 | H | 0 |
| | MOTA | | N SER H | | 35.147 | 36.126 | 5.074 | 1.00 44.47 | H | N |
| 15 | ATOM | | CA SER H | 52 | 35.938 | 35.254 | 4.277 | 1.00 47.09 1.00 46.84 | H H | C |
| | MOTA | | CB SER H | | 36.368 | 34.010 33.304 | 5.034 5.485 | 1.00 47.85 | H | ŏ |
| | MOTA | | OG SER H | | 35.231 35.147 | $33.304 \\ 34.674$ | 3.405 | 1.00 47.49 | H | Ċ |
| | ATOM | | C SER F | | 33.926 | 34.918 | 2.875 | 1.00 45.99 | Н | 0 |
| 00 | MOTA MOTA | 5053 5054 | O SER I | | 35.865 | 33.884 | 2.201 | 1.00 49.05 | H | N |
| 20 | ATOM | | CA SER I | | 35.209 | 33.375 | 0.894 | 1.00 49.67 | H | C C |
| | ATOM | 5056 | CB SER F | | 36.168 | 32.723 | -0.041 | 1.00 49.00 1.00 50.01 | H H | Ö |
| | MOTA | 5057 | OG SER I | | 36.770 | 31.610 32.332 | $0.686 \\ 1.448$ | 1.00 50.01 1.00 50.73 | H | č |
| | MOTA | 5058 | C SER I | | 34.185 33.092 | 32.140 | 0.880 | 1.00 51.07 | H | 0 |
| 25 | ATOM ATOM | 5059 5060 | O SER I | | 34.403 | 31.912 | 2.647 | 1.00 51.03 | H | N |
| | ATOM | 5061 | CA GLY | | 33.540 | 30.925 | 3.220 | 1.00 52.23 | H | C |
| | ATOM | 5062 | C GLY | H 54 | 32.454 | 31.432 | 4.040 | 1.00 53.84 1.00 54.98 | H H | C |
| | MOTA | 5063 | O GLY | | 31.664 | 30.683 | $4.614 \\ 4.172$ | 1.00 54.98 | H | N |
| 30 | MOTA | 5064 | N GLY | | 32.326 31.281 | 32.712 33.279 | 5.125 | 1.00 55.93 | H | C |
| | ATOM | 5065 5066 | CA GLY | | 31.653 | 33.592 | 6.603 | 1.00 56.90 | H | С |
| | ATOM ATOM | 5067 | O GLY | | 30.829 | 34.053 | 7.401 | 1.00 59.08 | H | 0 |
| | ATOM | 5068 | N ASN | н 56 | 32.901 | 33.390 | 7.042 | 1.00 56.97 1.00 56.87 | H H | N C |
| 35 | MOTA | 5069 | CA ASN | | 33.241 | 33.813 33.311 | 8.376 8.686 | 1.00 56.87 1.00 58.57 | H | č |
| | ATOM | 5070 | CB ASN CG ASN | | 34.641 34.848 | 31.707 | 8.674 | 1.00 60.80 | H | C |
| | MOTA MOTA | 5071 5072 | CG ASN OD1 ASN | | 35.948 | 31.265 | 8.259 | 1.00 62.91 | H | 0 |
| | ATOM | 5072 | ND2 ASN | | 33.932 | 30.944 | 9.202 | 1.00 58.88 | H | N |
| 40 | MOTA | 5074 | C ASN | | 33.328 | 35.349 | 8.488 | 1.00 56.17 1.00 56.06 | H H | C |
| | MOTA | 5075 | O ASN | | 33.756 | 35.993 | 7.536 9.651 | 1.00 55.51 | H | N |
| | MOTA | 5076 | N THR | | 32.945 32.817 | 35.940 37.327 | 9.817 | 1.00 53.59 | H | C |
| | MOTA | 5077 5078 | CA THR CB THR | | 31.419 | | 10.158 | 1.00 53.48 | H | C |
| 45 | MOTA ATOM | 5079 | OG1 THR | | 30.924 | 37.625 | 11.595 | 1.00 52.48 | H | 0 |
| 40 | ATOM | 5080 | CG2 THR | | 30.394 | | 9.249 | 1.00 51.25 | H H | C |
| | MOTA | 5081 | C THR | | 33.855 | | 10.893 11.883 | 1.00 53.43 1.00 52.41 | H | ŏ |
| | ATOM | 5082 | O THR | | 34.062 34.453 | | 10.713 | 1.00 52.67 | H | N |
| F0 | MOTA MOTA | 5083 5084 | N TYR CA TYR | | 35.398 | | 11.668 | 1.00 52.76 | H | C |
| 50 | ATOM | 5085 | CB TYR | | 36.725 | 39.194 | 11.145 | 1.00 52.49 | H | C C |
| | MOTA | 5086 | CG TYR | | 37.059 | | 10.726 9.504 | 1.00 53.52 1.00 53.54 | H H | C |
| | MOTA | 5087 | CD1 TYR | | 36.701 | | 9.099 | 1.00 53.34 | H | Č |
| | MOTA | 5088 | CE1 TYR CD2 TYR | | 37.013 37.868 | | 11.533 | 1.00 53.39 | H | C |
| 55 | MOTA ATOM | 5089 5090 | CD2 TYR CE2 TYR | | 38.229 | 35.741 | 11.070 | 1.00 54.38 | H | C |
| | ATOM | 5091 | CZ TYR | | 37.748 | 35.425 | 9.790 | | H | C C |
| | MOTA | 5092 | OH TYR | н 58 | 38.058 | | 9.344 | | H H | C |
| | MOTA | 5093 | C TYR | | 35.244 35.056 | | 11.935 10.975 | | Н | ŏ |
| 60 | MOTA | 5094 | O TYR | | 35.26 | | 13.182 | 1.00 52.51 | H | N |
| | MOTA | 5095 5096 | N TYR CA TYR | | 34.99 | | 13.523 | 1.00 52.95 | H | C |
| | MOTA MOTA | 5097 | CB TYR | | 33.53 | 3 43.018 | 14.083 | | H | C |
| | ATOM | 5098 | CG TYR | н 59 | 32.41 | | 13.081 13.231 | | H H | C |
| 65 | ATOM | 5099 | CD1 TYR | | 31.793 30.86 | | 13.231 12.405 | | Н | С |
| | MOTA | 5100 5101 | CE1 TYR CD2 TYR | | 31.99 | | 12.072 | 1.00 54.68 | H | С |
| | ATOM ATOM | | | | 31.04 | 9 42.822 | 11.166 | 1.00 55.81 | H | C |
| | MOTA | | | | 30.49 | 4 41.541 | 11.353 | 1.00 55.91 | H | С |
| | | | | | 252 | | | | | |

| | | 29.437 41.021 10.587 1.00 56.18 | н О |
|-----|--|--|------------|
| | ATOM 5104 OH TYR H 59 ATOM 5105 C TYR H 59 | 35.873 43.285 14.582 1.00 52.14 | н С н О |
| | ATOM 5106 O TYR H 59 | 36 301 44 578 14.540 1.00 51.10 | H N |
| 5 | ATOM 5108 CD PRO H 60 | 35.948 45.627 13.547 1.00 50.32 | н С н С |
| J | ATOM 5109 CA PRO H 60 | 37.619 46.481 15.123 1.00 50.61 | H C |
| | ATOM 5111 CG PRO H 60 | 36.550 46.883 14.122 1.00 49.50 | н С н С |
| | ATOM 5112 C PRO H 60 | 34.753 45.912 16.527 1.00 51.38 | н О |
| 10 | ATOM 5114 N ASP H 61 | 36.342 45.820 18.000 1.00 53.47 | H N H C |
| | ATOM 5115 CA ASP H 61 ATOM 5116 CB ASP H 61 | 36.206 46.275 20.452 1.00 55.46 | н С н С |
| | ATOM 5117 CG ASP H 61 | 36.538 44.902 20.885 1.00 57.77 37.403 44.611 21.711 1.00 58.30 | н О |
| 15 | ATOM 5118 OD1 ASP H 61 ATOM 5119 OD2 ASP H 61 | 35.804 44.026 20.420 1.00 58.83 | н О н С |
| | ATOM 5120 C ASP H 61 | 34.655 47.507 19.054 1.00 54.65 33.545 47.569 19.547 1.00 54.74 | н О |
| | ATOM 5121 O ASP H 61 ATOM 5122 N SER H 62 | 35.102 48.381 18.162 1.00 54.82 | H N H C |
| 20 | ATOM 5123 CA SER H 62 | 34.543 49.676 17.993 1.00 56.32 35.638 50.516 17.192 1.00 57.39 | н С |
| | ATOM 5124 CB SER H 62 ATOM 5125 OG SER H 62 | 35.889 50.046 15.798 1.00 59.78 | н О Н С |
| | ATOM 5126 C SER H 62 | 33.163 49.619 17.362 1.00 56.10 32.468 50.520 17.414 1.00 55.34 | H O |
| 0.5 | ATOM 5127 O SER H 62 ATOM 5128 N VAL H 63 | 32.900 48.597 16.552 1.00 56.41 | H N H C |
| 25 | ATOM 5129 CA VAL H 63 | 31.699 48.386 15.847 1.00 56.65 31.890 48.550 14.285 1.00 55.76 | н С |
| | ATOM 5130 CB VAL H 63 ATOM 5131 CG1 VAL H 63 | 32.652 49.663 14.056 1.00 54.30 | н С н С |
| | ATOM 5132 CG2 VAL H 63 | 32.541 47.542 15.005 1.00 57.66 | н С |
| 30 | ATOM 5133 C VAL H 63 ATOM 5134 O VAL H 63 | 29.946 46.678 15.567 1.00 57.57 | H O H N |
| | ATOM 5135 N LYS H 64 | 31 037 44 767 17.007 1.00 60.19 | н С |
| | ATOM 5136 CA LYS H 64 ATOM 5137 CB LYS H 64 | 31.873 43.826 17.908 1.00 61.48 | н С н С |
| 35 | ATOM 5138 CG LYS H 64 | 32 299 41 554 18.817 1.00 64.36 | н С |
| | ATOM 5139 CD LYS H 64 ATOM 5140 CE LYS H 64 | 31.942 40.092 19.153 1.00 65.73 | H C H N |
| | ATOM 5141 NZ LYS H 64 | 32.676 33.341 27.722 1.00 60.59 | н с |
| 40 | ATOM 5142 C LYS H 64 ATOM 5143 O LYS H 64 | 29.431 45.586 18.780 1.00 62.28 | H O H N |
| 40 | ATOM 5144 N GLY H 65 | 27 365 44 166 17.600 1.00 58.63 | н С |
| | ATOM 5145 CA GLY H 65 ATOM 5146 C GLY H 65 | 26.533 45.288 17.147 1.00 58.62 | н С н О |
| | ATOM 5147 O GLY H 65 | 27 108 46.269 16.463 1.00 57.07 | H N |
| 45 | ATOM 5148 N ARG H 66 ATOM 5149 CA ARG H 66 | 26.280 47.247 15.780 1.00 55.77 | н С н С |
| | ATOM 5150 CB ARG H 66 | 26 000 48 903 17.660 1.00 53.21 | н С |
| | ATOM 5152 CD ARG H 66 | 27.229 50.369 17.891 1.00 51.58 | H C H N |
| 50 | ATOM 5153 NE ARG H 66 | 28.931 51.813 16.823 1.00 50.26 | н С |
| | ATOM 5155 NH1 ARG H 66 | 28.037 52.565 16.279 1.00 48.61 | f H N |
| | ATOM 5156 NH2 ARG H 66 | 26.389 47.081 14.297 1.00 55.54 | н С |
| 55 | ATOM 5158 O ARG H 66 | 25.503 47.441 13.635 1.00 55.80 | H O H N |
| | ATOM 5159 N PHE H 67 | 27.672 46.501 12.322 1.00 54.62 | . н С |
| | ATOM 5161 CB PHE H 67 | 29.029 47.046 11.863 1.00 55.55 | н С |
| | ATOM 5162 CG PHE H 67 | 28 315 49.397 12.535 1.00 54.88 | н С |
| 60 | ATOM 5164 CD2 PHE H 67 | 30.137 49.156 11.059 1.00 55.35 | н С н С |
| | ATOM 5165 CE1 PHE H 67 | 30.283 50.503 11.012 1.00 55.27 | н С |
| | ATOM 5167 CZ PHE H 67 | 29.510 51.315 11.687 1.00 55.25 | н С н С |
| 65 | ATOM 5168 C PHE H 67 | 27.967 44.187 12.703 1.00 53.47 | н О |
| | ATOM 5170 N THR H 68 | 27.185 44.863 10.716 1.00 53.47 | H N H C |
| | ATOM 5171 CA THR H 68 | 27.043 43.466 10.208 1.00 54.52 25.623 42.863 10.372 1.00 55.50 | н С |
| | ATOM 5172 CB THR H 68 | 253 | |

| ANTOM 5175 C THR H 68 26.25 44.268 8.008 1.00 54.03 H CO STOR STOR STOR STOR STOR STOR STOR STO | | " ATOM | 5173 5174 | OG1 THR | | | 25.227 25.626 | 42.726 41.324 | 9.847 | 1.00 56.3 1.00 54. | 74 | H H | 0 0 |
|--|----|--------|--------------|----------|---------|---|------------------|------------------|----------|-----------------------|--------------|--------|--------|
| ATOM 5147 0 N. T. S. | | ATOM | 5175 | C THR | н 68 | | 27.369 | | | 1.00 54.0 | | | C 0 |
| ATOM 5178 CR LIE H 69 28.8971 42.515 6.983 1.00 51.28 H CO ATOM 5180 CG2 LIE H 69 31.330 42.476 7.476 7.476 7.497 1.00 50.24 H CO ATOM 5181 CG1 LIE H 69 31.035 42.476 7.476 7.476 7.497 1.00 50.24 H CO ATOM 5181 CG1 LIE H 69 31.035 42.206 5.358 1.00 49.67 H CO ATOM 5181 CG1 LIE H 69 28.260 41.291 6.305 1.00 51.26 H CO ATOM 5185 CO SER H 70 27.863 41.288 5.093 1.00 50.529 H CO ATOM 5186 CA SER H 70 27.863 41.288 5.093 1.00 50.53 H CO ATOM 5187 CB SER H 70 27.863 41.288 5.093 1.00 50.55 H DO ATOM 5188 CS SER H 70 27.7607 40.193 2.895 1.00 51.59 H CO ATOM 5189 CS SER H 70 27.7607 40.193 2.895 1.00 51.69 H CO ATOM 5189 CS SER H 70 27.7607 40.193 2.895 1.00 51.69 H CO ATOM 5193 CS SER H 70 27.7607 40.193 2.895 1.00 51.69 H CO ATOM 5192 CA ARG H 71 27.821 39.220 0.685 1.00 51.92 H CO ATOM 5193 CS ARG H 71 27.821 39.220 0.685 1.00 51.92 H CO ATOM 5194 CG ARG H 71 27.821 39.220 0.685 1.00 51.92 H CO ATOM 5195 CD ARG H 71 29.280 37.000 59.665 1.00 50.87 H CO ATOM 5195 CD ARG H 71 29.280 37.000 59.665 1.00 50.87 H CO ATOM 5195 CD ARG H 71 27.821 39.220 0.685 1.00 50.87 H CO ATOM 5195 CD ARG H 71 29.280 37.000 0.965 1.00 50.87 H CO ATOM 5196 CD ARG H 71 29.280 37.000 0.965 1.00 50.87 H CO ATOM 5190 CD ARG H 71 29.280 37.000 0.965 1.00 50.87 H CO ATOM 5190 CD ARG H 71 29.280 37.000 0.965 1.00 50.87 H CO ATOM 5190 CD ARG H 71 29.280 37.000 0.965 1.00 50.80 H CO ATOM 5190 CD ARG H 71 29.280 37.000 0.965 1.00 50.80 H CO ATOM 5190 CD ARG H 71 | 5 | | | | | | 28.418 | 42.758 | 8.312 | 1.00 52. | 81 | | N |
| ATOM 5180 CG2 ILE H 69 ATOM 5181 CG1 LIE H 69 ATOM 5182 CG1 LIE H 69 ATOM 5182 CG1 LIE H 69 ATOM 5182 CG1 LIE H 69 ATOM 5183 C LIE H 69 ATOM 5184 O LIE H 69 ATOM 5185 C LIE H 69 ATOM 5186 C LIE H 70 ATOM 5186 C LIE H 70 ATOM 5187 C LIE H 70 ATOM 5187 C LIE H 70 ATOM 5188 C LIE H 70 ATOM 5189 C LIE H 70 ATOM 5191 N ARG H 71 ATOM 5191 N ARG H 71 ATOM 5192 C ARG H 71 ATOM 5192 C ARG H 71 ATOM 5193 CB ARG H 71 ATOM 5193 CB ARG H 71 ATOM 5195 CD ARG H 71 ATOM 5196 C ARG H 71 ATOM 5197 C ARG H 71 ATOM 5198 C C ARG H 71 ATOM 5199 C C ARG H 71 ATOM 5199 C C ARG H 71 ATOM 5190 C ARG H 71 ATOM 5190 C C | 3 | MOTA | 5178 | CA ILE | н 69 | | | | | 1.00 51. | 28 | H | C |
| ATOM 5182 CD1 ILLE H 69 | | | | CG2 ILE | н 69 | | 31.062 | 41.283 | | | | | C C |
| No. St. | 40 | | | | | | | | 5.195 | 1.00 49. | 96 | H | C |
| ATOM 5184 O LIE H 97 | 10 | | 5183 | C ILE | н 69 | | 28.280 | | | 1.00 51. | 26 09 | | 0 |
| ATOM 5186 CA SER FO 27.401 40.072 4.393 1.00 51.00 | | | | | | | | 41.288 | 5.093 | 1.00 50. | 56 | | N |
| APOING Sar Color Ser H TO 25,366 41,376 4,072 1,00 51,90 H Color APOING Sar TO 27,707 40,193 2,895 1,00 51,69 H Color APOING 5190 O Ser H TO 28,045 41,274 2,444 1,00 51,39 H Color APOING 5192 Ca ARG H TO 27,528 39,135 2,133 1,00 51,78 H TO APOING 5193 CB ARG H TO 29,163 39,135 2,133 1,00 51,78 H TO APOING 5193 CB ARG H TO 29,163 38,500 0,369 1,00 50,83 H Color APOING 5194 CG ARG H TO 29,163 38,500 0,369 1,00 50,83 H Color APOING 5195 CD ARG H TO 30,574 36,465 0,945 1,00 47,051 H APOING 5196 NE ARG H TO 30,574 36,465 0,945 1,00 47,051 H APOING 5196 NE ARG H TO 31,331 36,661 -0,344 1,00 47,051 H APOING 5196 NE ARG H TO 32,635 36,755 -0,514 1,00 44,25 H APOING 5198 NH1 ARG H TO 33,442 36,645 0,445 0,00 0,444 1,00 44,25 H APOING 5199 NH2 ARG H TO 33,437 36,861 -1,231 1,00 44,25 H APOING S198 NH1 ARG H TO 33,437 36,861 -1,231 1,00 44,25 H APOING S198 NH1 ARG H TO 26,269 37,400 0,00 | | MOTA | 5186 | CA SER | н 70. | | | | | 1.00 50. | 53 | | C |
| ATOM 5189 C SER H 70 27.707 40.193 2.8045 1.00 51.39 H 70 ATOM 5190 O SER H 70 28.045 41.274 2.444 1.00 51.39 H 71 27.528 39.135 2.133 1.00 51.78 H 10 ATOM 5191 N ARG H 71 27.528 39.135 2.133 1.00 51.78 H 10 ATOM 5192 CA ARG H 71 29.280 37.000 0.969 1.00 50.83 H 61 ATOM 5193 CB ARG H 71 29.280 37.000 0.969 1.00 50.83 H 61 ATOM 5195 CD ARG H 71 30.574 36.65 0.945 1.00 47.03 H 10 ATOM 5195 CD ARG H 71 30.574 36.65 0.945 1.00 47.03 H 10 ATOM 5195 CD ARG H 71 30.574 36.65 0.945 1.00 47.03 H 10 ATOM 5197 CZ ARG H 71 32.653 6.659 -0.514 1.00 47.03 H 10 ATOM 5197 CZ ARG H 71 32.653 6.659 -0.514 1.00 42.99 H 10 ATOM 5199 NH2 ARG H 71 32.636 6.659 -0.544 1.00 42.99 H 10 ATOM 5199 NH2 ARG H 71 32.636 861 -0.344 1.00 42.99 H 10 ATOM 5199 NH2 ARG H 71 32.636 861 -0.344 1.00 52.00 H 10 ATOM 5201 C ARG H 71 26.794 97.742 1.00 42.99 H 10 ATOM 5201 C ARG H 71 26.794 97.742 1.00 52.00 H 10 ATOM 5202 N ASP H 72 26.756 38.087 -2.065 1.00 52.00 H 10 ATOM 5203 CA ASP H 72 25.750 38.087 -2.065 1.00 54.30 H 10 ATOM 5203 CA ASP H 72 25.750 38.087 -2.065 1.00 54.30 H 10 ATOM 5205 CG ASP H 72 23.5811 38.605 -3.544 1.00 57.72 H 10 ATOM 5205 CG ASP H 72 23.5811 37.685 -4.373 1.00 63.22 H 10 ATOM 5206 CD ARG H 72 24.706 39.144 -2.484 1.00 57.72 H 10 ATOM 5205 CG ASP H 72 23.5811 37.685 -4.373 1.00 63.54 H 10 ATOM 5207 CD ARG H 72 26.756 39.184 -3.631 1.00 53.35 H 10 ATOM 5207 CD ARG H 72 26.756 39.184 -3.631 1.00 53.35 H 10 ATOM 5208 C ASP H 72 26.756 39.184 -3.631 1.00 53.35 H 10 ATOM 5208 C ASP H 72 26.756 39.184 -3.631 1.00 53.35 H 10 ATOM 5208 C ASP H 72 26.756 39.184 -3.631 1.00 53.35 H 10 ATOM 5211 CA ARG H 73 26.751 36.267 -3.230 1.00 53.35 H 10 ATOM 5212 CA ARG H 73 26.756 ATOM 5206 CD ARG H 73 26.756 ATOM 5208 CA ASP H 72 26.756 ATOM 5208 CA ASP | 15 | | | | н 70 | | 25.366 | 41.376 | 4.072 | 1.00 51. | 90 | | C |
| ATOM 5191 N ARG H 71 27,528 39,135 2.133 1.00 51.78 H C ATOM 5192 CA ARG H 71 27,821 39,220 0.685 1.00 51.92 H C ARG H 71 29,163 38,500 0.369 1.00 50.83 H C ARG H 71 29,163 38,500 0.369 1.00 50.83 H C ARG H 71 29,163 38,500 0.369 1.00 48.57 H C ARG H 71 29,163 38,500 0.369 1.00 48.57 H C ARG H 71 ARG H 71 30,574 36,465 0.945 1.00 47.03 H C ARG H 71 30,574 36,465 0.945 1.00 47.03 H C ARG H 71 31,331 36,661 -0.344 1.00 43,91 H C ARG H 71 31,331 36,661 -0.344 1.00 43,91 H C ARG H 71 31,331 36,661 -0.344 1.00 44,20 H C ARG H 71 32,635 36,759 -0.514 1.00 44,20 H C ARG H 71 32,635 36,759 -0.514 1.00 44,20 H C ARG H 71 32,635 36,759 -0.514 1.00 44,20 H C ARG H 71 32,635 36,759 -0.514 1.00 44,20 H C ARG H 71 32,433 36,645 -0.485 1.00 44,20 H C ARG H 71 32,433 36,645 -0.485 1.00 44,20 H C ARG H 71 32,435 36,645 -1.721 1.00 42,20 H C ARG H 71 32,435 36,645 -1.721 1.00 42,20 H C ARG H 71 32,435 36,645 -1.721 1.00 42,20 H C ARG H 71 32,435 36,645 -1.721 1.00 42,20 H C ARG H 71 32,435 36,645 -1.721 1.00 42,20 H C ARG H 71 32,435 36,645 -1.721 1.00 42,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,20 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,63 H C ARG H 71 32,435 37,435 4 -1.255 1.00 54,63 H C ARG H 71 32,435 37,435 4 -1.255 1.00 53,45 H C ARG H 71 32,445 37,45 H C ARG H 71 32,445 37,4 | | MOTA | 5189 | C SER | н 70 | | | | | 1.00 51. | 39 | H | 0 |
| ATOM 5192 CA ARG H 71 | | | | N ARG | H 71 | | 27.528 | 39.135 | 2.133 | 1.00 51. | .78 92 | | N C |
| ATOM 5194 CC ARG H 71 29,280 37.000 0.946 1.00 47.03 H 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 | 20 | MOTA | | | | | 27.821 29.163 | | 0.369 | 1.00 50. | . 83 | H | С |
| ATOM 5195 NE ARG H 71 31.331 36.661 -0.344 1.00 44.40 H H 6 ATOM 5197 CZ ARG H 71 32.635 36.759 -0.514 1.00 44.40 H H 6 ATOM 5198 NH1 ARG H 71 33.437 36.861 -0.344 1.00 44.40 H H 6 ATOM 5198 NH1 ARG H 71 33.443 36.645 0.485 1.00 44.25 H 1 ATOM 5199 NH2 ARG H 71 33.437 36.861 -1.721 1.00 42.99 H 1 ATOM 5200 C ARG H 71 26.269 37.442 0.575 1.00 52.40 H 1 ATOM 5201 O ARG H 71 26.269 37.442 0.575 1.00 52.40 H 1 ATOM 5202 N ASP H 72 26.636 38.752 -1.253 1.00 53.22 H 1 ATOM 5203 CA ASP H 72 26.636 38.752 -1.253 1.00 53.22 H 1 ATOM 5205 CG ASP H 72 24.706 39.144 -2.484 1.00 61.26 H 1 ATOM 5205 CG ASP H 72 24.706 39.144 -2.484 1.00 61.26 H 1 ATOM 5205 CG ASP H 72 23.581 38.605 -3.544 1.00 61.26 H 1 ATOM 5205 CG ASP H 72 23.881 37.685 -4.373 1.00 63.54 H 1 ATOM 5205 CG ASP H 72 23.581 38.605 -3.544 1.00 63.54 H 1 ATOM 5205 CG ASP H 72 23.881 37.685 -4.373 1.00 63.54 H 1 ATOM 5205 CG ASP H 72 23.881 37.685 -4.373 1.00 63.54 H 1 ATOM 5205 CG ASP H 72 26.466 38.104 -3.544 1.00 61.26 H 1 ATOM 5207 OD2 ASP H 72 26.756 38.360 -4.373 1.00 63.54 H 1 ATOM 5208 C ASP H 72 26.756 38.360 -4.373 1.00 63.54 H 1 ATOM 5210 N ASN H 73 26.711 36.267 -3.230 1.00 53.35 H 1 ATOM 5210 N ASN H 73 26.711 36.267 -3.230 1.00 53.35 H 1 ATOM 5211 CA ASN H 73 26.711 36.267 -3.230 1.00 53.35 H 1 ATOM 5212 CB ASN H 73 28.264 34.510 -3.344 1.00 52.96 H 1 ATOM 5213 CG ASN H 73 29.674 35.743 -2.461 1.00 56.11 H 1 ATOM 5216 C ASN H 73 29.674 35.743 -2.461 1.00 56.19 H 1 ATOM 5217 O ASN H 73 29.674 35.743 -2.461 1.00 56.19 H 1 ATOM 5218 N ALA H 74 25.09 35.601 -7.134 1.00 53.76 H 1 ATOM 5218 N ALA H 74 25.09 35.601 -7.134 1.00 53.76 H 1 ATOM 5218 N ALA H 74 25.09 35.601 -7.134 1.00 53.96 H 1 ATOM 5218 N ALA H 74 25.09 35.601 -7.134 1.00 53.97 H 1 ATOM 5221 CB ALA H 74 24.963 35.601 -7.134 1.00 53.96 H 1 ATOM 5222 CB ALA H 74 24.963 35.601 -7.134 1.00 53.96 H 1 ATOM 5221 CB ALA H 74 25.09 35.601 -7.134 1.00 53.96 H 1 ATOM 5222 CB ALA H 74 25.048 36.940 -7.773 1.00 53.96 H 1 ATOM 5223 N ALA H 74 25.048 36.940 -7.773 1.00 53.94 H 1 ATOM 5223 N ALA H 74 25.048 | | | 5194 | CG ARG | н 71 | | 29.280 | | | 1.00 48. | . 57 . 03 | | C |
| 25 ATOM 5197 CZ ARG H 71 32.635 36.759 -0.514 1.00 44.425 H 71 ATOM 5198 NH1 ARG H 71 33.433 36.635 -0.596 1.00 44.25 H 71 ATOM 5199 NH2 ARG H 71 33.433 36.861 -1.721 1.00 44.25 H 71 ATOM 5199 NH2 ARG H 71 26.794 38.435 0.008 1.00 52.40 H 71 26.794 38.435 0.008 1.00 52.40 H 71 26.794 38.435 0.008 1.00 52.40 H 72 26.636 38.752 -1.253 1.00 53.02 H 72 25.750 38.087 -2.065 1.00 52.00 H 72 72 72 72 72 72 72 72 72 72 72 72 72 | | | | CD ARG | | | | 36.661 | -0.344 | 1.00 43 | .91 | | N C |
| ATOM 5199 Nill ARG H 71 26.794 38.435 0.008 1.00 52.40 H H ATOM 5201 C ARG H 71 26.269 37.442 0.575 1.00 52.40 H H ATOM 5201 O ARG H 71 26.269 37.442 0.575 1.00 52.00 H H ATOM 5202 N ASP H 72 25.750 38.087 -2.065 1.00 53.22 H H ATOM 5204 CB ASP H 72 25.750 38.087 -2.065 1.00 54.30 H ATOM 5204 CB ASP H 72 24.706 33.144 -2.484 1.00 57.72 H ATOM 5206 ODI ASP H 72 23.881 37.665 -4.373 1.00 63.54 H ATOM 5206 ODI ASP H 72 23.881 37.665 -4.373 1.00 63.54 H ATOM 5208 C ASP H 72 23.881 37.665 -4.373 1.00 63.54 H ATOM 5208 C ASP H 72 26.491 37.583 -3.244 1.00 61.12 H ATOM 5208 C ASP H 72 26.491 37.583 -3.244 1.00 53.96 H ATOM 5210 N ASN H 73 26.756 38.60 -4.270 1.00 54.68 H ATOM 5211 CA ASN H 73 27.576 35.773 -4.308 1.00 53.42 H ATOM 5212 CB ASN H 73 28.264 34.501 -3.899 1.00 53.42 H ATOM 5212 CB ASN H 73 29.674 35.743 -2.461 1.00 53.42 H ATOM 5212 CB ASN H 73 29.674 35.743 -2.461 1.00 53.42 H ATOM 5212 CB ASN H 73 29.674 35.743 -2.461 1.00 53.45 H ATOM 5212 CB ASN H 73 29.674 35.743 -2.461 1.00 53.45 H ATOM 5212 CB ASN H 73 29.674 35.743 -2.461 1.00 53.797 H ATOM 5215 ND2 ASN H 73 29.674 35.743 -2.461 1.00 53.797 H ATOM 5215 ND2 ASN H 73 29.674 35.743 -2.461 1.00 55.11 H ATOM 5217 O ASN H 73 29.674 35.743 -2.461 1.00 53.76 H ATOM 5218 N ALA H 74 24.963 35.601 -5.830 1.00 53.76 H ATOM 5218 N ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C ALA H 74 25.008 36.940 -7.773 1.00 53.48 H ATOM 5221 C ALA H 74 25.008 36.940 -7.773 1.00 53.48 H ATOM 5222 CB ARG H 75 23.861 40.024 -6.712 1.00 53.48 H ATOM 5223 N ARG H 75 22.486 39.9266 -7.416 1.00 53.48 H ATOM 5221 C ALA H 74 25.008 36.940 -7.773 1.00 53.48 H ATOM 5222 CB ARG H 75 23.861 40.024 -6.712 1.00 53.48 H ATOM 5223 N ARG H 75 22.486 39.9266 -7.416 1.00 53.48 H ATOM 5220 CB ALA H 74 25.008 36.940 -7.731 1.00 53.48 H ATOM 5221 C ALA H 74 25.008 37.960 -6.946 1.00 53.48 H ATOM 5222 CB ARG H 75 22.486 39.9266 -7.416 1.00 53.48 H ATOM 5222 CB ARG H 75 22.486 39.9266 -7.416 1.00 53.48 H ATOM 5220 CB ARG H 75 22.486 39 | 25 | ATOM | 5197 | CZ ARG | ; н 71 | | 32.635 | | | 1.0044 1.0044 | .40 .25 | | N |
| ATOM 5201 O ARG H 71 26.794 38.443 0.006 1.00 52.00 H ARG H 71 26.269 37.442 0.575 1.00 52.00 H ARG H 71 26.269 37.442 0.575 1.00 53.202 H ARG H 71 26.269 37.442 0.575 1.00 53.202 H ARG H 71 26.269 37.442 0.575 1.00 53.202 H ARG H 72 25.750 38.087 -2.065 1.00 54.30 H ARG H 72 25.750 38.087 -2.065 1.00 54.30 H ARG H 72 24.706 39.144 -2.484 1.00 57.72 H ARG H 72 25.581 38.608 -3.544 1.00 57.72 H ARG H 72 25.581 38.608 -3.544 1.00 51.26 H ARG H 72 23.881 37.685 -4.373 1.00 61.12 H ARG H 72 26.756 38.3605 -3.544 1.00 61.26 H ARG H 72 26.756 38.360 -4.270 1.00 54.68 H ARG H 72 26.756 38.360 -4.270 1.00 54.68 H ARG H 72 26.756 38.360 -4.270 1.00 54.68 H ARG H 72 26.756 38.360 -4.270 1.00 54.68 H ARG H 73 26.756 38.360 -4.270 1.00 53.42 H ARG H 73 26.756 38.360 -4.270 1.00 53.42 H ARG H 73 26.756 38.360 -4.270 1.00 53.42 H ARG H 73 27.576 35.773 -4.308 1.00 53.42 H ARG H 73 28.64 34.501 -3.899 1.00 53.42 H ARG H 73 28.64 34.501 -3.899 1.00 53.42 H ARG H 74 28.64 34.501 -3.899 1.00 53.42 H ARG H 74 28.64 34.501 -3.899 1.00 52.96 H ARG H 75 213 CB ARS H 73 29.265 33.639 -1.842 1.00 53.97 H ARG H 75 215 CB ARG H 75 22.26 ARG H 75 22.36 ARG H 74 24.963 35.601 -7.134 1.00 52.70 H ARG H 75 221 CB ARG H 74 25.137 37.023 -8.944 1.00 53.76 H ARG H 75 221 CB ARG H 75 22.466 39.956 -7.445 1.00 53.88 H 75 222 C ARG H 75 22.486 39.956 -7.445 1.00 53.88 H 75 22.486 39.956 -7.445 1.00 53.84 H 75 22.486 39.956 -7.445 1.00 53.84 H 75 22.486 39.956 -7.445 1.00 53.88 H 75 22.486 39.956 -7.445 | | | | | | | 33.137 | 36.861 | -1.721 | 1.00 42 | .99 | | N C |
| 30 ATOM 5203 CA ASP H 72 | | MOTA | 5200 | | | | | | | 1.00 52 | .00 | H | 0 |
| ATOM 5204 CB ASP H 72 23.581 38.605 -3.544 1.00 61.26 H ATOM 5205 CG ASP H 72 23.581 38.605 -3.544 1.00 61.26 H ATOM 5205 CD ASP H 72 23.581 38.605 -3.544 1.00 61.26 H ATOM 5207 CD ASP H 72 22.466 39.184 -3.613 1.00 63.54 H ATOM 5208 C ASP H 72 22.466 39.184 -3.613 1.00 63.54 H ATOM 5209 O ASP H 72 26.756 38.360 -4.270 1.00 53.96 H ATOM 5210 N ASN H 73 26.711 36.267 -3.230 1.00 53.35 H ATOM 5211 CA ASN H 73 27.576 35.773 -4.308 1.00 53.35 H ATOM 5212 CB ASN H 73 27.576 35.773 -4.308 1.00 52.96 H ATOM 5212 CB ASN H 73 27.576 35.773 -4.308 1.00 52.96 H ATOM 5213 CG ASN H 73 29.674 35.743 -2.461 1.00 56.11 H ATOM 5215 C ASN H 73 29.674 35.743 -2.461 1.00 53.97 H ATOM 5216 C ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5216 C ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5217 O ASN H 73 27.701 35.344 -6.643 1.00 52.43 H ATOM 5218 N AIA H 74 24.963 35.601 -7.134 1.00 52.70 H ATOM 5218 N AIA H 74 24.963 35.601 -7.134 1.00 53.07 H ATOM 5210 CA AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5220 CB AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5222 C AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5220 CB AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C AIA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5220 CB AIA H 74 24.966 37.960 -6.946 1.00 53.48 H ATOM 5222 C AIA H 74 25.028 9.266 -7.416 1.00 53.48 H ATOM 5222 C AIA H 74 25.028 9.266 -7.416 1.00 53.48 H ATOM 5222 C AIA H 74 25.028 9.266 -7.416 1.00 53.48 H ATOM 5222 C AIA H 75 22.486 39.946 -7.773 1.00 53.07 H ATOM 5222 C AIA H 75 22.486 39.946 -7.416 1.00 53.76 H ATOM 5223 C AIA H 74 25.028 9.266 -7.416 1.00 53.48 H ATOM 5222 C AIA H 75 22.486 39.946 -7.7173 1.00 53.01 H ATOM 5222 C AIA H 75 26.956 40.070 -7.320 1.00 53.01 H ATOM 5223 C AIA H 75 22.486 39.946 -7.445 1.00 56.70 H ATOM 5223 C AIA H 75 22.486 39.946 -7.416 1.00 50.79 H ATOM 5223 C AIA H 75 22.486 39.946 -7.416 1.00 50.38 H ATOM 5223 C AIA H 75 22.486 39.946 -7.416 1.00 50.79 H AT | 30 | | | N ASI | Р Н 72 | | 26.636 | 38.752 | | | | | N C |
| ATOM 5206 ODI ASP H 72 23.581 38.605 -3.544 1.00 61.20 H ATOM 5207 OD2 ASP H 72 22.466 39.184 -3.613 1.00 63.54 H ATOM 5207 OD2 ASP H 72 22.466 39.184 -3.613 1.00 63.54 H ATOM 5209 O ASP H 72 26.491 37.583 -3.244 1.00 53.96 H ATOM 5209 O ASP H 72 26.756 38.360 -4.270 1.00 54.68 H ATOM 5210 N ASN H 73 26.711 36.267 -3.230 1.00 53.35 H ATOM 5211 CA ASN H 73 26.711 36.267 -3.230 1.00 53.42 H ATOM 5211 CB ASN H 73 28.264 34.501 -3.899 1.00 52.96 H ATOM 5212 CB ASN H 73 29.163 34.664 -2.695 1.00 54.63 H ATOM 5214 ODI ASN H 73 29.674 35.743 -2.461 1.00 56.11 H ATOM 5215 ND2 ASN H 73 29.674 35.743 -2.461 1.00 56.11 H ATOM 5216 C ASN H 73 29.245 33.639 -1.842 1.00 53.97 H ATOM 5217 O ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5218 N ALA H 74 25.709 35.801 -7.134 1.00 53.76 H ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 C ALA H 74 25.048 39.956 -7.445 1.00 57.90 H ATOM 5222 C ARG H 75 23.861 40.024 -6.712 1.00 53.84 H ATOM 5222 C ARG H 75 23.861 40.024 -6.712 1.00 53.98 H ATOM 5222 C ARG H 75 23.861 40.024 -6.712 1.00 53.98 H ATOM 5222 C ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 C ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 C ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5231 NEW ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5233 O ARG H 75 22.486 39.956 -7.445 1.00 50.79 H ATOM 5233 O ARG H 75 22.486 39.956 -7.445 1.00 50.79 H ATOM 5233 O ARG H 75 22.486 39.956 -7.445 1.00 50.79 H ATOM 5233 O ARG H 75 22.486 39.956 -7.445 1.00 50.79 H ATOM 5233 O ARG H 75 22.486 39.956 -7.445 1.00 50.79 H ATOM 5233 O ARG H 75 22.486 39.9426 -7.732 1.00 50.04 H ATOM 5233 O ARG H 75 22.486 39.9426 -7.445 1.00 50.79 H ATOM 5234 N ARG H 75 22.486 39.9426 -7.918 1.00 | | MOTA | | | | | | | | 1.00 57 | .72 | H | C |
| ATOM 5200 OD1 ASP H 72 | | | 5205 | CG ASI | ⊋н 72 | | 23.581 | | | | | | C O |
| ATOM 5208 C ASP H 72 26.491 37.583 -3.424 1.00 53.35 H ATOM 5210 N ASN H 73 26.711 36.267 -3.230 1.00 53.35 H ATOM 5211 CA ASN H 73 27.576 38.360 -4.270 1.00 53.35 H ATOM 5211 CB ASN H 73 27.576 35.773 -4.308 1.00 53.42 H ATOM 5212 CB ASN H 73 28.264 34.501 -3.899 1.00 52.96 H ATOM 5213 CG ASN H 73 29.163 34.664 -2.695 1.00 56.11 H ATOM 5214 OD1 ASN H 73 29.245 33.639 -1.842 1.00 56.11 H ATOM 5215 ND2 ASN H 73 29.245 33.639 -1.842 1.00 55.11 H ATOM 5216 C ASN H 73 27.010 35.742 -5.731 1.00 52.70 H ATOM 5218 N ALA H 74 25.709 35.801 -5.830 1.00 53.07 H ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 53.07 H ATOM 5210 CB ALA H 74 24.963 35.164 -6.989 1.00 53.76 H ATOM 5220 CB ALA H 74 25.048 36.940 -7.773 1.00 53.76 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.76 H ATOM 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.76 H ATOM 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5223 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5224 CB ARG H 75 22.486 39.956 -7.445 1.00 56.70 H ATOM 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 56.70 H ATOM 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 66.38 H ATOM 5221 NH ARG H 75 19.499 39.885 -5.884 1.00 66.38 H ATOM 5223 NA ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 53.01 H ATOM 5231 NH2 ARG H 75 19.499 39.885 -5.884 1.00 66.38 H ATOM 5232 C ARG H 75 19.499 39.885 -5.884 1.00 66.38 H ATOM 5231 NH2 ARG H 75 19.499 39.885 -5.884 1.00 66.38 H ATOM 5232 C ARG H 75 26.491 41.234 -7.849 1.00 51.72 H ATOM 5231 NH2 ARG H 75 26.491 41.234 -7.849 1.00 51.72 H ATOM 5232 C ARG H 75 26.491 41.234 -7.849 1.00 50.07 H ATOM 5233 NH 76 29.563 37.982 -9.470 1.00 50.064 H ATOM 5233 NH 76 29.563 37.982 -9.470 1.00 50.064 H ATOM 5234 N ASN H 76 29.563 37.982 -9.470 1.00 50.064 H ATOM 5238 OD1 ASN H 76 29.563 37.982 -9.470 1.0 | 25 | | | OD1 ASI | | | | 39.184 | -3.613 | 1.00 63 | .54 | | 0 |
| ATOM 5210 N ASN H 73 26.711 36.267 -3.230 1.00 53.35 H ATOM 5211 CA ASN H 73 27.576 35.773 -4.308 1.00 53.42 H ATOM 5212 CB ASN H 73 28.264 34.501 -3.899 1.00 52.96 H ATOM 5213 CG ASN H 73 29.163 34.664 -2.695 1.00 54.63 H ATOM 5214 OD1 ASN H 73 29.674 35.743 -2.461 1.00 56.11 H ATOM 5215 ND2 ASN H 73 29.674 35.743 -2.461 1.00 56.11 H ATOM 5216 C ASN H 73 29.245 33.639 -1.842 1.00 53.97 H ATOM 5216 C ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5217 O ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5218 N ALA H 74 25.709 35.801 -5.830 1.00 53.07 H ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 53.07 H ATOM 5210 CB ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.84 H ATOM 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.84 H ATOM 5222 C CB ARG H 75 22.4946 37.960 -6.946 1.00 53.48 H ATOM 5222 C CB ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5226 CG ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5229 CZ ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5229 CZ ARG H 75 22.486 39.956 -7.4416 1.00 53.84 H ATOM 5229 CZ ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 C ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5223 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5230 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5230 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5231 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5232 C ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5233 N ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5231 N ARG H 75 22.486 39.916 -5.935 1.00 66.988 H ATOM 5232 C ARG H 75 22.486 39.916 -5.935 1.00 67.53 H ATOM 5232 C ARG H 75 22.486 39.916 -5.935 1.00 65.98 H ATOM 5233 N ARG H 75 22.486 39.916 -7.445 1.00 57.90 H ATOM 5233 N ARG H 75 26.355 40.00 70 -7.320 1.00 53.01 H ATOM 5234 N ARG H 75 26.355 40.00 70 -7.32 | 33 | MOTA | 5208 | C AS | РН 72 | | | | | | | | 0 |
| ## ATOM 5211 CA ASN H 73 27.576 35.773 -4.308 1.00 52.96 H ## ATOM 5212 CB ASN H 73 73 29.163 34.664 -2.695 1.00 54.63 H ## ATOM 5214 ODI ASN H 73 29.163 34.664 -2.695 1.00 54.63 H ## ATOM 5215 ND2 ASN H 73 29.1674 35.743 -2.461 1.00 53.97 H ## ATOM 5216 C ASN H 73 29.245 33.639 -1.842 1.00 53.97 H ## ATOM 5217 O ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ## ATOM 5218 CA ALA H 74 25.709 35.801 -5.830 1.00 53.07 H ## ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ## ATOM 5220 CB ALA H 74 25.048 36.940 -7.773 1.00 53.76 H ## ATOM 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ## ATOM 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.48 H ## ATOM 5222 CB ARG H 75 24.946 37.023 -8.944 1.00 53.84 H ## ATOM 5225 CB ARG H 75 25.028 39.266 -7.416 1.00 53.84 H ## ATOM 5226 CG ARG H 75 23.861 40.024 -6.712 1.00 57.90 H ## ATOM 5227 CD ARG H 75 21.361 40.798 -6.811 1.00 57.90 H ## ATOM 5228 NE ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ## ATOM 5228 NE ARG H 75 21.361 40.798 -6.811 1.00 67.53 H ## ATOM 5230 NH1 ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ## ATOM 5231 NH2 ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ## ATOM 5234 N ASN H 76 29.315 40.254 -7.918 1.00 50.79 H ## ATOM 5235 CA ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ## ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 50.64 H ## ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ## ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 50.64 H ## ATOM 5233 O ARG H 75 26.355 40.070 | | | | | | | 26.711 | 36.267 | -3.230 | 1.00 53 | .35 | | C N |
| ATOM 5212 CG ASN H 73 29.163 34.664 -2.695 1.00 54.63 H 29.163 34.664 -2.695 1.00 54.63 H 34.00 5214 OD1 ASN H 73 29.245 33.639 -1.842 1.00 53.97 H 34.00 5216 C ASN H 73 29.245 33.639 -1.842 1.00 52.70 H 35.072 ASN H 73 27.010 35.722 -5.731 1.00 52.70 H 34.00 5217 O ASN H 73 27.010 35.722 -5.731 1.00 52.43 H 34.00 5218 N ALA H 74 25.709 35.801 -5.830 1.00 53.07 H 34.00 5218 N ALA H 74 25.709 35.801 -5.830 1.00 53.07 H 34.00 5220 CB ALA H 74 23.449 35.164 -6.989 1.00 52.82 H 34.00 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H 34.00 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.98 H 34.00 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.98 H 34.00 5222 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H 34.00 5222 C ALA H 74 25.048 36.940 -7.473 1.00 53.348 H 34.00 5222 C ALA H 75 22.946 37.960 -6.946 1.00 53.48 H 34.00 5222 C ALA H 75 22.946 37.960 -6.946 1.00 53.48 H 34.00 5222 C ALA H 75 22.946 39.956 -7.446 1.00 53.48 H 34.00 5225 CB ARG H 75 22.486 39.956 -7.445 1.00 57.90 H 34.00 5225 CB ARG H 75 22.486 39.956 -7.445 1.00 57.90 H 34.00 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 60.38 H 34.00 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 60.38 H 34.00 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 60.38 H 34.00 5228 NE ARG H 75 22.486 39.956 -7.445 1.00 60.38 H 34.00 5228 NE ARG H 75 19.499 39.426 -5.935 1.00 65.98 H 34.00 5228 NE ARG H 75 19.499 39.426 -5.935 1.00 65.98 H 34.00 5223 NH1 ARG H 75 19.499 39.426 -5.935 1.00 67.53 H 34.00 5231 NH2 ARG H 75 26.355 40.070 -7.320 1.00 53.01 H 34.00 5234 N ASN H 76 26.355 40.070 -7.320 1.00 50.79 H 34.00 5234 N ASN H 76 26.491 41.234 -7.849 1.00 51.72 H 34.00 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.64 H 34.00 5237 N ASN H 76 29.315 40.254 -7.918 1.00 50.64 H 34.00 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 50.64 H 34.00 5241 O ASN H 76 29.563 37.982 -7.603 1.00 50.64 H 34.00 5241 O ASN H 76 29.563 37.982 -7.603 1.00 50.64 H 34.00 5241 O ASN H 76 29.563 37.982 -7.603 1.00 50.64 H 34.00 5241 O ASN H 76 29.563 37.982 -7.603 1.00 50.64 H 34.00 5241 O ASN H 76 29.563 37.982 -7. | | MOTA | 5211 | | | | | | | 1.00 52 | .96 | H | С |
| ATOM 5215 ND2 ASN H 73 29.674 33.639 -1.842 1.00 53.97 H ATOM 5215 ND2 ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5217 O ASN H 73 27.701 35.344 -6.643 1.00 52.43 H ATOM 5218 N ALA H 74 25.709 35.801 -5.830 1.00 53.07 H ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5210 CB ALA H 74 23.449 35.164 -6.989 1.00 53.76 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 C ALA H 74 25.137 37.023 -8.944 1.00 54.91 H ATOM 5223 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5224 CA ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5225 CB ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5226 CG ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5227 CD ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ATOM 5229 CZ ARG H 75 19.499 39.885 -5.884 1.00 64.88 H ATOM 5230 NH1 ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5231 NH2 ARG H 75 19.499 39.426 -5.935 1.00 67.53 H ATOM 5232 C ARG H 75 19.499 39.426 -5.935 1.00 67.53 H ATOM 5233 O ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 CA ASN H 76 27.361 39.476 -6.669 1.00 51.34 H ATOM 5233 CA ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5235 CA ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 50.88 H ATOM 5239 ND2 ASN H 76 29.731 38.958 -8.434 1.00 50.88 H ATOM 5230 ND2 ASN H 76 29.731 38.958 -8.434 1.00 50.88 H ATOM 5230 ND2 ASN H 76 29.731 38.958 -8.434 1.00 50.88 H ATOM 5230 ND2 ASN H 76 29.731 38.958 -8.434 1.00 50.64 H ATOM 5230 ND2 ASN H 76 29.731 38.958 -7.605 1.00 47.56 H | 40 | | | CG AS | N H 73 | | 29.163 | 34.664 | | | | | C O |
| ATOM 5216 C ASN H 73 27.010 35.722 -5.731 1.00 52.70 H ATOM 5217 O ASN H 73 27.701 35.344 -6.643 1.00 52.43 H ATOM 5218 N ALLA H 74 24.963 35.801 -5.830 1.00 53.07 H ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 52.76 H ATOM 5220 CB ALA H 74 23.449 35.164 -6.989 1.00 52.82 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 O ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5223 N ARG H 75 25.028 39.266 -7.416 1.00 53.84 H ATOM 5224 CA ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5225 CB ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5226 CG ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5227 CD ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5228 NE ARG H 75 20.699 39.885 -5.884 1.00 60.38 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5230 NH1 ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5231 NH2 ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5232 N ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 N ASN H 76 26.355 40.070 -7.320 1.00 53.01 H ATOM 5234 N ASN H 76 28.632 40.121 -6.877 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.79 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.313 38.958 -8.434 1.00 51.70 H ATOM 5230 C ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.68 H ATOM 5238 OD1 ASN H 76 29.315 37.982 -7.663 1.00 52.12 H ATOM 5230 C ASN H 76 29.563 37.982 -7.663 1.00 52.12 H ATOM 5230 C ASN H 76 29.563 37.982 -7.663 1.00 49.22 H ATOM 5231 O ASN H 76 29.563 37.982 -7.663 1.00 49.22 H ATOM 5234 O C ASN H 76 29.563 37.982 -7.663 1.00 49.22 H ATOM 5230 C ASN H 76 29.563 37.982 -7.663 1.00 49.22 H ATOM 5231 O ASN H 76 29.563 40.254 -7.918 1.00 50.64 H ATOM 5230 O C ASN H 76 29.563 40.254 -7.918 1.00 50.64 H ATOM 5230 O C ASN H 76 29.563 40.254 -7.918 1.00 50.64 H ATOM 5231 O ASN H 76 29.563 40.254 -7.918 1.00 50.64 H ATOM 5231 O ASN H 76 29.563 40.254 -7.9 | | MOTA | | | | | | | -1.842 | 1.00 53 | .97 | H | N |
| 45 ATOM 5218 N ALA H 74 25.770 35.801 -5.830 1.00 53.07 H ATOM 5219 CA ALA H 74 24.963 35.601 -7.134 1.00 53.76 H ATOM 5220 CB ALA H 74 23.449 35.164 -6.989 1.00 52.82 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5221 C ALA H 74 25.137 37.023 -8.944 1.00 54.91 H ATOM 5223 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5225 CB ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5225 CB ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5226 CG ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5227 CD ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ATOM 5228 NE ARG H 75 20.699 39.885 -5.884 1.00 64.88 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5231 NH2 ARG H 75 19.499 39.426 -5.935 1.00 67.53 H ATOM 5231 NH2 ARG H 75 19.499 39.426 -5.935 1.00 67.53 H ATOM 5232 C ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 O ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.34 H ATOM 5233 O ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 CA ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.79 H ATOM 5238 OD1 ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.315 40.254 -7.603 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.363 38.820 -9.470 1.00 50.64 H ATOM 5230 CA ASN H 76 29.315 40.254 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.368 42.494 -6.227 1.00 47.56 H | | | 5216 | C AS | N H 73 | | 27.010 | | | | | | С 0 |
| ATOM 5219 CA ALA H 74 24.963 35.661 -7.154 1.00 52.82 H ATOM 5220 CB ALA H 74 23.449 35.164 -6.989 1.00 52.82 H ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 O ALA H 74 25.137 37.023 -8.944 1.00 54.91 H ATOM 5223 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5224 CA ARG H 75 25.028 39.266 -7.416 1.00 53.84 H ATOM 5225 CB ARG H 75 22.486 39.956 -7.416 1.00 56.70 H ATOM 5226 CG ARG H 75 22.486 39.956 -7.445 1.00 56.70 H ATOM 5227 CD ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ATOM 5228 NE ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5230 NH1 ARG H 75 19.499 39.426 -5.935 1.00 67.53 H ATOM 5231 NH2 ARG H 75 19.147 38.611 -5.004 1.00 68.48 H ATOM 5232 C ARG H 75 26.491 41.234 -7.849 1.00 53.01 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.72 H ATOM 5234 N ASN H 76 26.491 41.234 -7.849 1.00 51.72 H ATOM 5235 CA ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ATOM 5238 OD1 ASN H 76 29.315 40.254 -7.918 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.731 38.958 -8.434 1.00 50.79 H ATOM 5230 OD1 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5237 CG ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5238 OD1 ASN H 76 29.966 42.494 -6.227 1.00 47.56 H | 45 | | | | | | 25.709 | 35.801 | -5.830 | 1.00 53 | 3.07 | | C N |
| ATOM 5221 C ALA H 74 25.048 36.940 -7.773 1.00 53.98 H ATOM 5222 O ALA H 74 25.137 37.023 -8.944 1.00 54.91 H ATOM 5223 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5224 CA ARG H 75 25.028 39.266 -7.416 1.00 53.84 H ATOM 5225 CB ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5226 CG ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5227 CD ARG H 75 20.699 39.885 -5.884 1.00 64.88 H ATOM 5228 NE ARG H 75 20.699 39.885 -5.884 1.00 64.88 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5231 NH2 ARG H 75 18.646 39.712 -6.877 1.00 67.53 H ATOM 5231 NH2 ARG H 75 19.147 38.611 -5.004 1.00 68.48 H ATOM 5233 O ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5234 N ASN H 76 26.355 40.070 -7.320 1.00 53.01 H ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 50.88 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 50.64 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | MOTA | 5219 | CA AL | АН 74 | | | | | 1.00 52 | 2.82 | H | С |
| 50 ATOM 5222 O ALA H 74 25.137 37.963 -6.946 1.00 53.48 H ATOM 5223 N ARG H 75 24.946 37.960 -6.946 1.00 53.48 H ATOM 5224 CA ARG H 75 25.028 39.266 -7.416 1.00 53.84 H ATOM 5225 CB ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5226 CG ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5227 CD ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5228 NE ARG H 75 20.699 39.885 -5.884 1.00 64.88 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5230 NH1 ARG H 75 18.646 39.712 -6.877 1.00 67.53 H ATOM 5231 NH2 ARG H 75 19.147 38.611 -5.004 1.00 68.48 H ATOM 5232 C ARG H 75 26.355 40.070 -7.320 1.00 63.301 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.34 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.34 H ATOM 5235 CA ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.313 38.958 -8.434 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | | | C AL | а н 74 | | 25.048 | 36.940 | -7.773 | | 3.98 1.91 | | C O |
| ATOM 5224 CA ARG H 75 25.028 39.266 -7.416 1.00 53.84 H ATOM 5225 CB ARG H 75 23.861 40.024 -6.712 1.00 56.70 H ATOM 5226 CG ARG H 75 22.486 39.956 -7.445 1.00 57.90 H ATOM 5227 CD ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ATOM 5228 NE ARG H 75 20.699 39.885 -5.884 1.00 64.88 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5230 NH1 ARG H 75 18.646 39.712 -6.877 1.00 67.53 H ATOM 5231 NH2 ARG H 75 19.147 38.611 -5.004 1.00 68.48 H ATOM 5233 O ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 O ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5234 N ASN H 76 26.491 41.234 -7.849 1.00 51.34 H ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5238 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | 50 | MOTA | | | | | | | -6.946 | 1.00 53 | 3.48 | H | N |
| ATOM 5225 CB ARG H 75 ATOM 5226 CG ARG H 75 ATOM 5227 CD ARG H 75 ATOM 5228 NE ARG H 75 ATOM 5228 NE ARG H 75 ATOM 5228 NE ARG H 75 ATOM 5229 CZ ARG H 75 ATOM 5230 NH1 ARG H 75 ATOM 5231 NH2 ARG H 75 ATOM 5232 C ARG H 75 ATOM 5232 C ARG H 75 ATOM 5233 O ARG H 75 ATOM 5233 O ARG H 75 ATOM 5234 N ASN H 76 ATOM 5235 CA ASN H 76 ATOM 5236 CB ASN H 76 ATOM 5237 CG ASN H 76 ATOM 5238 OD1 ASN H 76 ATOM 5238 OD1 ASN H 76 ATOM 5239 ND2 ASN H 76 ATOM 5240 C ASN H 76 ATOM 5241 O ASN H 76 ATOM | | | 5224 | . CA AR | RG H 75 | | 25.028 | 39.266 | | _ | | | C |
| 55 ATOM 5227 CD ARG H 75 21.361 40.798 -6.811 1.00 60.38 H ATOM 5228 NE ARG H 75 20.699 39.885 -5.884 1.00 64.88 H ATOM 5229 CZ ARG H 75 19.499 39.426 -5.935 1.00 65.98 H ATOM 5231 NH2 ARG H 75 18.646 39.712 -6.877 1.00 67.53 H ATOM 5232 C ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.34 H ATOM 5234 N ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | | | | | | | 39.956 | -7.445 | 1.00 5 | 7.90 | | C |
| ATOM 5228 NE ARG H 75 ATOM 5229 CZ ARG H 75 ATOM 5230 NH1 ARG H 75 ATOM 5231 NH2 ARG H 75 ATOM 5231 NH2 ARG H 75 ATOM 5232 C ARG H 75 ATOM 5233 O ARG H 75 ATOM 5233 O ARG H 75 ATOM 5234 N ASN H 76 ATOM 5235 CA ASN H 76 ATOM 5236 CB ASN H 76 ATOM 5237 CG ASN H 76 ATOM 5238 OD1 ASN H 76 ATOM 5238 OD1 ASN H 76 ATOM 5239 ND2 ASN H 76 ATOM 5239 ND2 ASN H 76 ATOM 5239 ND2 ASN H 76 ATOM 5240 C ASN H 76 ATOM 5241 O ASN H 76 ATOM 5241 | 55 | MOTA | 5227 | CD AF | | | | | | _ | 4.88 | H | N |
| ATOM 5230 NH1 ARG H 75 18.646 39.712 -6.877 1.00 68.48 H ATOM 5231 NH2 ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.34 H ATOM 5234 N ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5239 ND2 ASN H 76 30.392 38.820 -9.470 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | | | | | | 19.499 | 39.426 | -5.935 | 1.00 6 | 5.98 | | C N |
| ATOM 5231 C ARG H 75 26.355 40.070 -7.320 1.00 53.01 H ATOM 5232 C ARG H 75 26.491 41.234 -7.849 1.00 51.34 H ATOM 5233 O ARG H 75 26.491 41.234 -7.849 1.00 51.72 H ATOM 5234 N ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5238 OD1 ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | MOTA | 5230 |) NH1 AF | | | | | | 1.00 6 | 8.48 | H | N |
| ATOM 5233 O ARG H 75 26.491 41.234 -7.043 1.00 51.72 H ATOM 5234 N ASN H 76 27.361 39.476 -6.669 1.00 51.72 H ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5238 OD1 ASN H 76 30.392 38.820 -9.470 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | 60 | | | C AI | RG H 75 | ; | 26.355 | 40.070 | -7.320 | 1.00 5 | 3.01 1 34 | | C |
| ATOM 5235 CA ASN H 76 28.632 40.121 -6.510 1.00 50.79 H ATOM 5236 CB ASN H 76 29.315 40.254 -7.918 1.00 50.88 H ATOM 5237 CG ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5238 OD1 ASN H 76 30.392 38.820 -9.470 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | MOTA | | | | | | | -6.669 | 1.00 5 | 1.72 | H | N |
| ATOM 5236 CB ASN H 76 29.315 40.234 -7.316 1.00 51.70 H ATOM 5237 CG ASN H 76 29.731 38.958 -8.434 1.00 51.70 H ATOM 5238 OD1 ASN H 76 30.392 38.820 -9.470 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | | | 5235 | CA A | SN H 76 | 5 | 28.632 | 2 40.123 | | | 0.79 0.88 | | C |
| ATOM 5238 OD1 ASN H 76 30.392 38.820 -9.470 1.00 50.64 H ATOM 5239 ND2 ASN H 76 29.563 37.982 -7.603 1.00 52.12 H ATOM 5240 C ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 H | 65 | | | | | | 29.733 | 1 38.958 | 8 -8.434 | 1.00 5 | 1.70 | | C |
| ATOM 5239 ND2 ASN H 76 28.444 41.544 -5.865 1.00 49.22 H ATOM 5240 C ASN H 76 28.444 41.544 -6.227 1.00 47.56 H ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.56 | 00 | ATOM | 5238 | 8 OD1 A | SN H 76 | | | | | 3 1.00 5 | 2.12 | H | N |
| ATOM 5241 O ASN H 76 29.086 42.494 -6.227 1.00 47.30 M | | | | | SN H 7 | 5 | 28.44 | 4 41.54 | 4 -5.865 | 5 1.00 4 | 9.22 | | C |
| OEA | | | | | | 5 | 29.08 | 6 42.49 | 4 -0.22 | , 1.00 4 | .,.50 | | Ü |

| | | | | | 27.729 | 41.553 | -4.754 | 1.00 47.69 | н | | N |
|----|--------------|--------------------|----------------------|------------------|------------------|----------------------|------------------|--------------------------|--------------|--------|--------|
| | MOTA | 5242 N 5243 CA | | 77 77 | 27.729 | 42.653 | -3.929 | 1.00 47.93 | H | | C C |
| | MOTA MOTA | 5244 CB | ILE H | 77 | 26.126 26.040 | 43.102 44.411 | -3.973 -3.140 | 1.00 47.80 1.00 48.14 | H | , | C |
| _ | MOTA | 5245 CG 5246 CG | · | 77 77 | 25.721 | 43.638 | -5.331 | 1.00 46.37 | H | | C C |
| 5 | ATOM ATOM | 5247 CD | 1 ILE H | 77 | 24.173 | 43.842 | -5.549 -2.487 | 1.00 45.88 1.00 48.54 | H L H | | C |
| | ATOM | 5248 C | ILE H ILE H | 77 7 7 | 27.998 27.825 | 42.386 41.270 | -1.957 | 1.00 48.81 | L H | | 0 |
| | ATOM ATOM | 5249 O 5250 N | LEU H | 78 | 28.610 | 43.389 | -1.863 | 1.00 47.84 1.00 48.57 | 1 H 7 H | | N C |
| 10 | ATOM | 5251 CA | | 78 | 29.059 30.563 | 43.294 43.649 | -0.509 -0.495 | 1.00 48.73 | , 3 H | | č |
| | MOTA | 5252 CF 5253 CG | | 78 78 | 31.088 | 43.596 | 0.929 | 1.00 47.6 | 7 H | | C |
| | ATOM ATOM | 5254 CI | D1 LEU H | 78 | 31.187 | 42.158 | 1.519 | 1.00 47.04 1.00 47.5 | 4 H 7 H | | C |
| | MOTA | 5255 CI | D2 LEU H | 78 78 | 32.365 28.299 | 44.371 44.319 | $1.207 \\ 0.352$ | 1.00 49.23 | 1 H | | C |
| 15 | MOTA | 5256 C 5257 O | | 78 78 | 27.826 | 45.315 | -0.052 | 1.00 50.4 | 5 H 5 H | | N |
| | MOTA ATOM | 5258 N | TYR H | 79 | 28.035 | 44.033 44.855 | 1.553 2.317 | 1.00 50.7 1.00 52.0 | 6 H | | C |
| | MOTA | 5259 C | | 79 79 | 27.177 25.742 | 44.140 | 2.498 | 1.00 53.3 | 5 H | | C |
| 20 | MOTA MOTA | 5260 CI 5261 C | | 79 79 | 24.871 | 43.972 | 1.172 | 1.00 55.8 1.00 56.5 | 7 H 1 H | | C |
| 20 | MOTA | 5262 C | D1 TYR H | 79 | 24.578 23.735 | 42.710 42.556 | 0.663 -0.481 | 1.00 57.9 | _ | | C |
| | MOTA | | E1 TYR H D2 TYR H | 79 79 | 24.374 | 45.043 | 0.491 | 1.00 55.7 | 2 H | | C |
| • | ATOM ATOM | | E2 TYR H | 79 | 23.572 | 44.882 | -0.639 -1.054 | 1.00 56.3 1.00 58.4 | 1 H | | C |
| 25 | MOTA | _ | Z TYR H | 79 79 | 23.247 22.609 | 43.650 43.533 | -2.252 | 1.00 60.1 | .2 F | Ī | 0 |
| | MOTA MOTA | 5267 O 5268 C | H TYR H | 79 | 27.702 | 45.191 | 3.633 | 1.00 52.1 1.00 51.2 | | | C O |
| | MOTA | 5269 C | TYR H | 79 | 28.365 27.289 | 44.358 46.360 | $4.266 \\ 4.152$ | 1.00 51.2 1.00 52.1 | | | N |
| | MOTA | 5270 N 5271 C | LEU H | 80 80 | 27.203 | 46.718 | 5.521 | 1.00 52.7 | 72 I | Į | C |
| 30 | MOTA MOTA | | CB LEU H | 80 | 28.802 | 47.563 | 5.493 6.905 | 1.00 51.0 1.00 52.4 |)5 1 14 I | I I | C C |
| | MOTA | | CG LEU H | 80 80 | 29.222 29.699 | 48.078 46.925 | 7.713 | 1.00 53.2 | 20 1 | H | С |
| | MOTA MOTA | 5274 C | CD1 LEU H | 80 | 30.226 | 49.254 | 7.078 | 1.00 51.8 | | H H | C |
| 35 | ATOM | 5276 | C LEU H | 80 | 26.405 25.923 | 47.402 48.431 | 6.180 5.665 | 1.00 53.0 | 00 | H | 0 |
| | MOTA | - - · · | O LEU H | 80 81 | 25.772 | 46.703 | 7.112 | 1.00 54. | 52 | H | N |
| | MOTA ATOM | | CA GLN H | 81 | 24.604 | | 7.836 8.221 | 1.00 55. 1.00 56. | 69 62 | H H | C C |
| | MOTA | 5280 | CB GLN H CG GLN H | 81 81 | 23.568 22.383 | 46.125 46.533 | | 1.00 58. | 33 | H | C |
| 40 | ATOM ATOM | | CG GLN H | 81 | 21.423 | 47.264 | 8.251 | 1.00 60. 1.00 62. | 67 40 | H H | C O |
| | ATOM | 5283 | OE1 GLN H | | 20.972 21.387 | 46.664 48.608 | | 1.00 62. | | H | N |
| | MOTA | | NE2 GLN H C GLN H | 81 81 | 25.055 | 47.763 | 9.110 | 1.00 56. | 82 | H | C O |
| 45 | MOTA MOTA | | O GLN H | 81 | 25.683 | | 9.959 9.331 | 1.00 57. 1.00 58. | 28 | H H | И |
| | MOTA | 5287 | N MET H | | 24.641 25.021 | | | 1.00 60. | 26 | H | C |
| | MOTA MOTA | | CB MET H | | 25.707 | 7 51.079 | 10.003 | 1.00 61. | 16 go | H H | C C |
| | MOTA | 5290 | CG MET H | 82A | 26.924 27.898 | 1 50.877 3 52.390 | 9.024 8.755 | 1.00 64. | 38 | H | s |
| 50 | MOTA | | SD MET H | | 27.093 | 1 52.775 | 7.376 | 1.00 62. | 45 | H | C C |
| | MOTA MOTA | | C MET H | 82A | 23.82 | | | | 13 | H H | ŏ |
| | MOTA | | O MET H | | 22.829 24.01 | | | 1.00 60. | . 07 | H | N |
| 55 | MOTA MOTA | | N SER H | | 22.88 | 0 50.393 | 3 13.477 | | | H H | C |
| 33 | ATOM | 5297 | CB SER F | 1 82B | 22.14 22.90 | | | | .61 | H | 0 |
| | MOTA | | OG SER F | | 23.44 | 9 51.10 | 8 14.761 | 1.00 60 | . 67 | H H | C O |
| | MOTA ATOM | | O SER I | 1 82B | 24.66 | 9 51.13 | | | . 39 . 07 | H | И |
| 60 | ATOM | 5301 | N SER I | | 22.63 23.17 | 5 51.84 4 52.80 | | 3 1.00 61 | .07 | H | C |
| | MOTA MOTA | | CA SER I | | 23.47 | 5 52.03 | 2 17.784 | | .29 | H H | C O |
| | ATOM | I 5304 | OG SER | H 82C | 22.61 | 9 50.93 7 53.60 | | | .65 | H | č |
| | ATOM | | C SER | | 24.37 25.33 | | 3 16.938 | 3 1.00 61 | .63 | H | O |
| 65 | MOTA MOTA | | N LEU | H 82D | 24.35 | 3 54.23 | 5 14.973 | | .41 .72 | H H | N C |
| | MOTA | 5308 | CA LEU | н 82D | 25.43 24.97 | | | 6 1.00 60 | .37 | H | C |
| | MOTA MOTA | | CB LEU | | 24.97 | | | | .24 | H | С |
| | AION | . 5510 | | | 255 | | | | | | |

| 5 10 15 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 5312 5313 5314 5315 5316 5317 5318 5319 5320 5321 5322 5323 5324 5325 5326 5327 5328 | CD1 LEU H CD2 LEU H C LEU H O LEU H N ARG H CA ARG H CB ARG H CG ARG H CD ARG H NE ARG H CZ ARG E NH1 ARG E NH2 ARG H O ARG H NH2 ARG H O ARG | 83 83 83 83 83 83 83 83 83 83 83 83 84 84 84 | 24.386 26.461 25.685 24.718 26.928 27.286 28.035 28.089 28.592 28.362 29.251 30.408 28.944 28.077 28.596 29.007 29.129 29.598 | 55.079 54.225 56.273 56.901 57.669 57.275 55.693 55.263 53.883 52.934 53.145 51.726 58.597 58.597 59.837 60.920 61.963 | 10.897 11.718 15.489 15.988 15.850 16.671 17.953 18.182 19.516 19.942 19.356 20.407 15.795 14.720 16.310 15.511 16.249 17.500 | 1.00 57.43 1.00 58.39 1.00 62.71 1.00 64.10 1.00 63.66 1.00 64.35 1.00 67.33 1.00 69.20 1.00 72.23 1.00 73.34 1.00 73.99 1.00 74.45 1.00 64.00 1.00 63.76 1.00 63.40 1.00 62.76 1.00 64.95 | нннннннннннннн | СССИСИСИСИСОИСО |
|---------------|--|--|---|--|--|--|--|--|-----------------------|------------------|
| 20 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 5329 5330 5331 5332 5333 5334 | C SER I O SER I N GLU I CA GLU I | H 84 H 84 H 85 H 85 H 85 | 30.367 30.796 31.008 32.356 32.818 | 60.434 60.790 59.642 59.037 58.098 | 15.059 13.908 15.944 15.635 16.798 | 1.00 62.17 1.00 62.05 1.00 60.48 1.00 59.67 1.00 59.83 1.00 63.33 | Н Н Н Н Н | C O N C C |
| 25 | ATOM ATOM ATOM ATOM ATOM | 5335 5336 5337 5338 5339 | CG GLU I CD GLU I OE1 GLU I OE2 GLU I C GLU I | н 85 н 85 н 85 н 85 | 32.602 31.403 31.387 30.602 32.385 | 58.833 58.378 57.224 59.226 58.092 | 17.959 18.752 19.125 19.061 14.494 14.307 | 1.00 63.33 1.00 64.36 1.00 65.15 1.00 66.28 1.00 58.39 1.00 59.02 | н н н н н | 00000 |
| 30 | ATOM ATOM ATOM ATOM ATOM | 5340 5341 5342 5343 5344 | O GLU N ASP CA ASP CB ASP CG ASP | н 86 н 86 н 86 н 86 | 33.412 31.253 31.158 29.880 30.017 | 57.539 57.774 56.814 55.991 54.951 | 13.908 12.864 13.036 14.084 14.834 | 1.00 56.08 1.00 54.11 1.00 55.33 1.00 57.05 1.00 58.36 | H H H H | и С С |
| 35 | ATOM ATOM ATOM ATOM ATOM | 5345 5346 5347 5348 5349 | C ASP | н 86 н 86 н 86 н 87 | 29.030 31.050 31.243 31.339 31.286 | 54.963 54.210 57.475 56.836 58.783 | 14.375 11.489 10.413 11.579 | 1.00 55.58 1.00 52.34 1.00 50.01 1.00 49.59 1.00 48.63 | H H H H | и О С |
| 40 | ATOM ATOM ATOM ATOM ATOM | 5350 5351 5352 5353 5354 | CA THR CB THR OG1 THR CG2 THR C THR | н 87 н 87 н 87 н 87 | 31.325 31.069 29.737 31.250 32.614 | 59.669 61.194 61.382 62.306 59.471 | 10.417 10.922 11.522 9.903 9.751 | 1.00 48.91 1.00 50.30 1.00 48.84 1.00 47.71 | н н н н н | 00000 |
| 45 | ATOM ATOM ATOM ATOM ATOM | 5355 5356 5357 5358 5359 | O THR N ALA CA ALA CB ALA C ALA | H 88 H 88 H 88 | 33.651 32.525 33.696 34.219 33.423 | 58.565 | 10.363 8.444 7.656 8.177 6.266 5.872 | 1.00 45.93 1.00 45.98 1.00 44.66 1.00 43.85 1.00 44.68 1.00 45.79 | н н н н | иссо |
| 50 | ATOM ATOM ATOM ATOM ATOM | 5360 5361 5362 5363 5364 | | H 89 H 89 H 89 H 89 | 32.260 34.498 34.488 35.704 35.662 | 58.433 57.827 58.347 57.806 | 5.474 4.173 3.419 1.922 | 1.00 44.08 1.00 43.11 1.00 43.90 1.00 45.35 | н н н н н | 2 C C Z |
| 55 | ATOM ATOM ATOM ATOM ATOM | 5365 5366 5367 5368 5369 | CE MET O MET N TYR | H 89 H 89 H 90 | 34.197 34.716 34.666 35.591 33.626 | 59.894 56.305 55.858 55.528 | 0.371 4.331 4.896 4.007 | 1.00 45.97 1.00 44.27 1.00 44.18 1.00 43.97 | H H H H | С О И С |
| 60 | ATOM ATOM ATOM ATOM ATOM | 5370 5371 5372 5373 5374 | CA TYR CB TYR CG TYR CD1 TYR CE1 TYR | H 90 H 90 H 90 H 90 | 33.576 32.153 31.822 32.069 31.778 31.543 | 53.648 53.774 52.770 52.890 | 4.374 5.899 6.771 8.105 6.446 | 1.00 42.74 1.00 42.49 1.00 42.71 1.00 41.99 1.00 41.28 | Н Н Н Н | 0000 |
| 65 | MOTA MOTA MOTA MOTA | 5378 | CE2 TYR CZ TYR OH TYR | . н 90 . н 90 . н 90 | 31.376 31.502 31.430 34.062 | 55.175 2 54.125 54.157 | 7.823 8.653 7 10.018 | 1.00 41.04 1.00 41.54 1.00 41.11 | н н н н | C C C |

| | | | mvn II | 90 | 33.501 | 53.708 | 1.596 1 | 00 44.77 | H | 0 |
|----|--------------|--------------------|----------------------|----------|------------------|-------------------|----------------------|--------------------------|----------|--------|
| | ATOM ATOM | 5380 O 5381 N | TYR H TYR H | 91 | 35.160 | 52.733 | | L.00 42.96 L.00 43.91 | H H | N C |
| | ATOM | 5382 CA | TYR H | 91 | 35.638 | 52.127 52.315 | 1.436 1 1.356 1 | L.00 43.91 L.00 42.41 | H | C |
| | MOTA | 5383 CB | TYR H | 91 91 | 37.214 37.761 | 53.729 | 1.202 | L.00 43.94 | H | C |
| 5 | MOTA | 5384 CG 5385 CD | TYR H 1 TYR H | 91 | 38.374 | 54.490 | | 1.00 41.91 | H | C |
| | ATOM ATOM | 5385 CD | | 91 | 38.708 | 55.820 | | 1.00 44.39 1.00 42.91 | H H | C C |
| | ATOM | 5387 CD | 2 TYR H | 91 | 37.789 | 54.267 · 55.415 · | -0.090 : -0.312 : | 1.00 45.60 | H | Ċ |
| | MOTA | 5388 CE | | 91 91 | 38.185 38.807 | 56.203 | 0.666 | 1.00 46.11 | H | C |
| 10 | MOTA | 5389 CZ 5390 OH | | 91 | 39.168 | 57.455 | | 1.00 50.45 | H H | C C |
| | MOTA MOTA | 5390 OII 5391 C | TYR H | 91 | 35.356 | 50.634 | | 1.00 44.70 1.00 43.09 | H H | 0 |
| | MOTA | 5392 0 | TYR H | 91 | 35.516 | 49.860 50.127 | 2.407 0.237 | 1.00 45.69 | H | N |
| | MOTA | 5393 N | CYS H | 92 92 | 35.128 35.005 | 48.670 | 0.074 | 1.00 46.10 | H | C |
| 15 | ATOM | 5394 CA 5395 C | CYS H | 92 92 | 36.380 | 48.319 | | 1.00 44.52 | H | C O |
| | ATOM ATOM | 5395 C 5396 O | CYS H | 92 | 36.965 | 48.974 | | 1.00 43.72 1.00 47.38 | H H | C |
| | ATOM | 5397 CE | CYS H | 92 | 34.031 | 48.498 46.885 | -1.175 -1.690 | 1.00 47.30 | H | S |
| | ATOM | 5398 SG | CYS H | 92 93 | 33.784 36.773 | 47.126 | -0.042 | 1.00 43.35 | H | N |
| 20 | ATOM | 5399 N 5400 CA | ALA H ALA H | 93 | 38.079 | 46.581 | -0.608 | 1.00 43.49 | H H | C C |
| | MOTA ATOM | 5400 CF | | 93 | 39.256 | 46.935 | 0.540 | 1.00 41.94 1.00 43.78 | H | C |
| | MOTA | 5402 C | ALA H | 93 | 38.022 | 45.117 44.409 | -0.627 0.487 | 1.00 45.76 | H | 0 |
| | MOTA | 5403 O | ALA H | 93 94 | 37.485 38.862 | 44.628 | -1.461 | 1.00 43.45 | H | N |
| 25 | MOTA | 5404 N 5405 C | ARG H A ARG H | 94 | 39.053 | 43.214 | -1.645 | 1.00 44.26 | H H | C |
| | MOTA MOTA | 5406 CI | | 94 | 39.576 | 42.862 | -3.109 -3.350 | 1.00 45.24 1.00 46.44 | H | č |
| | MOTA | 5407 C | G ARG H | 94 | 39.501 39.929 | 41.398 40.954 | -3.330 -4.994 | 1.00 47.28 | H | C |
| | MOTA | 5408 C | | 94 94 | 41.337 | 40.997 | -5.159 | 1.00 49.70 | H | N |
| 30 | MOTA | 5409 N 5410 C | | 94 | 41.991 | 40.672 | -6.278 | 1.00 50.40 | H H | C N |
| | ATOM ATOM | • | H1 ARG H | 94 | 41.357 | 40.531 | -7.402 -6.311 | 1.00 50.46 1.00 46.10 | H | N |
| | ATOM | | H2 ARG H | 94 | 43.276 40.201 | 40.565 42.746 | -0.761 | 1.00 44.81 | H | C |
| | MOTA | 5413 C | | 94 94 | 41.240 | 43.215 | -0.817 | 1.00 45.02 | H | O |
| 35 | MOTA MOTA | 5414 O 5415 N | | | 39.932 | 41.776 | 0.081 | 1.00 44.55 | H H | N C |
| | MOTA | | A LEU H | 95 | 40.997 | 41.445 | $1.189 \\ 2.470$ | 1.00 43.74 1.00 41.49 | H | č |
| | MOTA | 5417 C | B LEU H | | 40.289 41.121 | 41.191 40.420 | 3.541 | 1.00 42.09 | H | C |
| | MOTA | | G LEU H D1 LEU H | | 42.374 | | 3.739 | 1.00 43.97 | H | C |
| 40 | MOTA MOTA | | D1 LEU H D2 LEU H | | 40.120 | 40.347 | 4.728 | 1.00 43.57 1.00 44.13 | H H | C |
| | ATOM | 5421 | | 95 | 41.584 | | $0.804 \\ 0.740$ | 1.00 44.13 | H | ŏ |
| | MOTA | 5422 | | | 40.903 42.765 | | 0.208 | 1.00 44.89 | H | N |
| | ATOM | 5423 N | N ASP H CA ASP H | | 43.557 | 39.273 | -0.364 | 1.00 45.30 | H | C |
| 45 | MOTA MOTA | | CB ASP H | <u>-</u> | 44.541 | . 39.676 | -1.408 | 1.00 44.92 1.00 48.16 | H H | C |
| | MOTA | 5426 | CG ASP F | I 96 | 43.888 | 40.051 | -2.741 -2.757 | 1.00 48.16 | H | Ö |
| | MOTA | 5427 (| OD1 ASP H | | 42.729 44.526 | | -3.840 | 1.00 49.25 | H | 0 |
| | MOTA | | OD2 ASP F C ASP F | | 44.212 | | 0.600 | 1.00 46.33 | H | C |
| 50 | MOTA MOTA | | O ASP I | | 44.551 | 1 37.315 | 0.197 | 1.00 48.00 1.00 46.28 | H H | N |
| | ATOM | | N GLY I | | 44.145 | | 1.933 2.935 | 1.00 45.80 | H | C |
| | MOTA | 5432 | CA GLY I | | 44.662 45.75 | | 3.889 | 1.00 46.63 | H | C |
| | ATOM | | O GLY I | | 46.43 | | 3.487 | 1.00 45.58 | H | N |
| 55 | MOTA MOTA | | N TYR | | 45.86 | 7 38.104 | 5.140 | 1.00 45.50 1.00 45.67 | , H H | C |
| | ATOM | | CA TYR | | 46.92 | | | | H | C |
| | MOTA | 5437 | CB TYR | | 46.87 47.03 | | | 1.00 45.01 | H | C |
| | ATOM | | CG TYR CD1 TYR | | 48.21 | | 7.805 | 1.00 45.57 | H | C C |
| 60 | MOTA MOTA | | CD1 TYR | | 48.41 | 8 34.646 | | | H H | C |
| | IOTA IOTA | | CD2 TYR | н 98 | 46.00 | | | | H | С |
| | ATO | 4 5442 | CE2 TYR | | 46.08 47.31 | | | | H | С |
| | IOTA | | CZ TYR OH TYR | | 47.43 | 9 32.515 | 7.945 | 1.00 47.02 | H | 0 |
| 65 | IOTA TOTA | | OH TYR C TYR | | 48.29 | 8 38.576 | 5.350 | 1.00 45.31 | H H | C |
| | OTA OTA | | O TYR | н 98 | 49.09 | | | | H | |
| | ATO! | M 5447 | N TYR | н 99 | 48.58 49.81 | | | | Н | |
| | OTA | | CA TYR | н 99 | | 57.02- | ,,,,, | | | |
| | | | | | 257 | | | | | |

| 5 | MOTA TOM ATOM ATOM ATOM ATOM ATOM ATOM | 5450 C 5451 C 5452 C 5453 C | CB TYR H 99 CG TYR H 99 CD1 TYR H 99 CE1 TYR H 99 CD2 TYR H 99 CE2 TYR H 99 | | 50.227 50.752 51.868 52.254 49.982 50.422 | 36.082 35.176 35.548 34.855 34.050 33.286 33.716 | 4.285 5.007 | 1.00 45.33 1.00 47.93 1.00 49.06 1.00 50.83 1.00 48.72 1.00 50.56 1.00 51.08 | H H H H H H | 0000000 |
|----|--|--|--|----------------------------------|--|--|---|--|----------------------------|---------------------------------------|
| 10 | MOTA MOTA MOTA MOTA MOTA MOTA | 5456 C 5457 C 5458 C 5459 P | O TYR H 99 N PHE H 100 | | 51.532 51.955 49.829 50.880 48.735 | 32.910 38.483 38.715 38.962 39.844 | 7.410 2.360 1.772 1.875 0.745 | 1.00 50.59 1.00 41.57 1.00 42.24 1.00 41.19 1.00 41.39 | H H H H | О О О |
| 15 | MOTA MOTA MOTA MOTA MOTA | 5461 (5462 (5463 (5464 (| CA PHE H 100 CB PHE H 100 CG PHE H 100 CD1 PHE H 100 CD2 PHE H 100 | A A A A | 48.715 47.950 48.520 48.087 49.650 | 39.136 37.790 36.764 37.668 35.463 | -0.406 -0.721 -0.162 -1.444 -0.394 | 1.00 41.14 1.00 40.31 1.00 39.72 1.00 39.59 1.00 40.58 | н н н н | מטטטט |
| 20 | ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 5466 5467 5468 5469 5470 | CE1 PHE H 100 CE2 PHE H 100 CZ PHE H 100 C PHE H 100 O PHE H 100 N GLY H 100 CA GLY H 100 | A A A A)A)B | 48.687 50.144 49.756 48.163 48.322 47.429 46.918 | 35.463 36.420 35.288 41.269 42.037 41.627 43.013 | -1.925 -1.187 0.851 -0.071 1.883 2.046 | 1.00 41.22 1.00 41.75 1.00 41.09 1.00 40.97 1.00 41.60 1.00 40.67 | н н н н н | C C C C C C C C C C C C C C C C C C C |
| 25 | ATOM ATOM ATOM ATOM | 5472 5473 5474 | C GLY H 100 O GLY H 100 N PHE H 100 CA PHE H 100 |)B)B)C)C | 45.530 44.855 45.087 43.876 | 43.259 42.360 44.491 44.969 | 1.366 0.912 1.365 0.745 | 1.00 41.06 1.00 40.75 1.00 39.30 1.00 39.10 1.00 36.63 | н н н н | C O N C C |
| 30 | MOTA MOTA MOTA MOTA MOTA | 5476 5477 5478 | CB PHE H 10 CG PHE H 10 CD1 PHE H 10 CD2 PHE H 10 CE1 PHE H 10 | 0C 0C 0C | 43.437 42.852 43.534 41.806 42.988 | 46.207 46.003 46.461 45.153 46.286 44.860 | 1.455 2.697 3.977 2.862 5.054 4.462 | 1.00 36.63 1.00 37.34 1.00 37.49 1.00 37.27 1.00 37.43 1.00 37.98 | н н н н | ממממ |
| 35 | MOTA ATOM ATOM ATOM ATOM ATOM | 5481 5482 5483 5484 5485 | CE2 PHE H 10 CZ PHE H 10 C PHE H 10 O PHE H 10 N ALA H 10 | 0C 0C 0C 1 | 41.256 41.775 44.310 44.856 44.112 44.715 | 45.401 45.386 46.558 44.508 44.704 | 5.277 -0.689 -0.957 -1.626 -2.982 | 1.00 38.05 1.00 38.92 1.00 37.99 1.00 38.37 1.00 38.04 | H H H 'H | C C O N |
| 40 | ATOM ATOM ATOM ATOM ATOM | 5486 5487 5488 5489 5490 | CA ALA H 10 CB ALA H 10 C ALA H 10 O ALA H 10 N TYR H 10 | 1 1 1 2 | 44.713 44.741 43.888 44.459 42.624 41.823 | 43.310 45.617 46.125 45.849 46.756 | -3.802 -3.860 -4.821 -3.587 -4.421 | 1.00 37.26 1.00 38.70 1.00 39.22 1.00 37.88 1.00 40.73 | H H H H | C N C |
| 45 | MOTA MOTA MOTA MOTA MOTA | 5491 5492 5493 5494 5495 | CA TYR H 10 CB TYR H 10 CG TYR H 10 CD1 TYR H 10 CE1 TYR H 10 | 2 2 2 2 | 40.881 41.770 42.487 43.463 | 45.940 45.485 44.255 43.807 | -5.415 -6.594 -6.486 -7.469 -7.510 | 1.00 43.71 1.00 46.39 1.00 46.61 1.00 47.40 1.00 46.31 | H H H H | I C I C |
| 50 | MOTA MOTA MOTA MOTA MOTA | 5496 5497 5498 5499 5500 | CD2 TYR H 10 CE2 TYR H 10 CZ TYR H 10 OH TYR H 10 C TYR H 10 |)2)2)2)2 | 42.176 43.139 43.697 44.665 40.807 | 45.953 44.635 44.236 47.551 | -8.505 -8.507 -9.426 -3.509 | 1.00 48.95 1.00 50.42 1.00 50.89 1.00 41.67 | H H H | H C |
| 55 | ATOM ATOM ATOM ATOM ATOM | 5501 5502 5503 5504 5505 | O TYR H 1 N TRP H 1 CA TRP H 1 CB TRP H 1 CG TRP H 1 |)3)3)3)3 | 40.259 40.625 39.717 40.386 41.471 | 48.838 49.645 50.618 50.174 | -2.117 -1.249 | 1.00 41.77 1.00 44.39 1.00 42.16 1.00 42.59 |]]] | H NH CH CH C |
| 60 | MOTA MOTA MOTA MOTA MOTA | 5506 5507 5508 5509 | CD2 TRP H 1 CE2 TRP H 1 CE3 TRP H 1 CD1 TRP H 1 NE1 TRP H 1 | 03 03 03 03 | 41.595 42.752 40.791 42.667 43.385 | 49.885 51.203 49.439 49.247 | 0.661 1.095 -1.605 -0.423 | 1.00 40.61 1.00 38.63 1.00 41.54 1.00 41.94 | | H CH CH NH CH |
| 65 | MOTA MOTA MOTA MOTA MOTA MOTA | 5511 5512 5513 5514 5515 5516 | CZ2 TRP H 1 CZ3 TRP H 1 CH2 TRP H 1 C TRP H 1 O TRP H 1 N GLY H 1 CA GLY H 1 | 03 03 03 03 03 04 | 43.179 41.257 42.429 38.809 39.069 37.600 | 7 51.321 9 50.777 5 50.440 8 50.687 3 50.646 | 2.447 2.818 3.949 -5.092 5.3.465 | 7 1.00 37.69 3 1.00 37.36 9 1.00 45.62 2 1.00 45.76 5 1.00 46.03 | | H C H C H C H O H N |
| | £11 O13 | | | | 258 | | | | | |

| | | | | | | | | | | | | | _ |
|----|--------------|--------------|----------|------------------------|------------|------------------|------------------|-------------------|-------|----------------------|--------|--------|--------|
| | ATOM | 5518 | | LY H 104 | 36. | | 52.969 | -3.990 | 1.00 | 50.39 50.04 | H H | | C O |
| | ATOM | 5519 | _ | LY H 104 LN H 105 | 37. 35. | | 53.342 53.812 | -3.435 -4.380 | 1.00 | 51.47 | н | | N |
| | ATOM ATOM | | | LN H 105 | 36. | | 55.263 | -4.372 | 1.00 | 53.77 | H H | | C C |
| 5 | ATOM | 5522 | CB G | LN H 105 | | 215 | 55.927 55.514 | -5.448 -6.818 | | 58.08 63.91 | H | | C |
| | ATOM | | | LN H 105 LN H 105 | | 012 577 | 56.078 | -7.031 | 1.00 | 67.40 | Н | | С |
| | ATOM ATOM | | OE1 G | LN H 105 | 37. | 891 | 57.324 | -6.794 | 1.00 | 70.51 68.61 | H H | | O N |
| , | MOTA | 5526 | | LN H 105 | | 506 541 | 55.151 55.826 | -7.495 -3.186 | 1.00 | 53.77 | H | | C |
| 10 | MOTA | | | LN H 105 LN H 105 | | 881 | 56.980 | -2.926 | 1.00 | 52.00 | H | | 0 |
| | MOTA MOTA | | N G | LY H 106 | 34. | 827 | 55.047 | -2.408 | | 53.76 53.09 | H H | | C N |
| | MOTA | 5530 | | LY H 106 | | .526 .100 | 55.500 56.020 | -1.099 -1.125 | 1.00 | 53.25 | H | | C |
| 45 | MOTA MOTA | | O G | LY Н 106 LY Н 106 | | 662 | 56.529 | -2.182 | 1.00 | 53.58 | H | | O |
| 15 | ATOM | 5533 | r n | THR H 107 | | .320 | 55.878 | $-0.055 \\ 0.001$ | 1.00 | 51.37 49.58 | H H | | C N |
| | MOTA | 5534 | | ГНR Н 107 ГНR Н 107 | | .068 .822 | 56.570 55.625 | -0.204 | 1.00 | 49.86 | H | | C |
| | MOTA MOTA | 5535 5536 | | THR H 107 | | .563 | 56.384 | -0.242 | | 52.01 | H H | | C |
| 20 | MOTA | 5537 | CG2 T | THR H 107 | | .563 | 54.703 57.202 | $0.994 \\ 1.297$ | | 48.32 49.76 | H | | C |
| | ATOM | 5538 | | THR H 107 THR H 107 | | .010 .356 | 56.588 | 2.303 | 1.00 | 49.74 | H | | 0 |
| | ATOM ATOM | 5539 5540 | N I | LEU H 108 | 30 | .618 | 58.471 | 1.346 | | 50.53 51.52 | H H | | C N |
| | ATOM | 5541 | | LEU H 108 | | .546, .711 | 59.237 60.734 | 2.619 2.383 | 1.00 | _ | н | | C |
| 25 | MOTA | 5542 5543 | | LEU H 108 LEU H 108 | | .064 | 61.420 | 2.162 | 1.00 | | H | | C |
| | MOTA MOTA | 5544 | CD1 | LEU H 108 | 32 | .029 | 62.939 | $1.777 \\ 3.414$ | 1.00 | 54.62 56.22 | H H | | C |
| | MOTA | 5545 | | LEU H 108 LEU H 108 | | .009 | 61.326 59.030 | 3.483 | 1.00 | 50.37 | H | | С |
| 30 | MOTA MOTA | 5546 5547 | | LEU H 108 | 28 | .272 | 59.085 | 2.998 | 1.00 | 48.78 | H H | | N O |
| 30 | MOTA | 5548 | N ' | VAL H 109 | | .532 | 58.955 58.808 | 4.786 5.695 | 1.00 |) 49.42) 50.40 | H | | C |
| | MOTA | 5549 5550 | CA CB | VAL H 109 VAL H 109 | | .471 | 57.421 | 6.360 | 1.00 | 50.35 | H | | C |
| | ATOM ATOM | 5550 5551 | CG1 | VAL H 109 | 27 | .558 | 57.361 | 7.473 | | 0 49.64 0 49.09 | H H | | C |
| 35 | MOTA | 5552 | | VAL H 109 | | 3.360 | 56.213 59.882 | 5.360 6.856 | | 0 51.56 | H | | С |
| | ATOM ATOM | 5553 5554 | C O | VAL H 109 VAL H 109 | | 611 | 59.948 | 7.554 | | 51.16 | ŀ | | N O |
| | ATOM | 5555 | N. | ALA H 110 | | 7.582 | 60.770 61.701 | 7.019 8.120 | 1.0 | 0 51.38 0 52.80 | I I | | C |
| | ATOM | 5556 | CA CB | ALA H 110 ALA H 110 | | 7.547 7.449 | 63.102 | 7.626 | 1.0 | 0 52.41 | Ŧ | | С |
| 40 | MOTA MOTA | 5557 5558 | CP | ALA H 110 | 2 | 5.460 | 61.441 | 9.110 | 1.0 | 0 52.98 0 52.47 | | I I | C O |
| | MOTA | 5559 | 0 | ALA H 110 | | 5.368 5.893 | 61.185 61.338 | 8.712 10.336 | 1.0 | 0 54.00 | | Ī | N |
| | MOTA MOTA | 5560 5561 | N CA | VAL H 111 VAL H 111 | | 6.075 | 61.036 | 11.455 | 1.0 | 0 55.55 | | F | C |
| 45 | MOTA | 5562 | CB | VAL H 111 | | 6.756 | | | 1.0 | 0 55.09 0 55.18 | | H H | C |
| | ATOM | 5563 | CG1 | VAL H 111 VAL H 111 | | 5.748 7.155 | | | 1.0 | 0 53.86 | | H | C |
| | ATOM ATOM | 5564 5565 | CGZ | VAL H 111 | 2 | 5.946 | 62.358 | 12.138 | | 0 57.61 0 57.50 | | H H | C O |
| | ATOM | 5566 | 0 | VAL H 111 | | 6.838 4.800 | | 12.773 11.987 | 1.0 | 0 59.58 | | H | N |
| 50 | MOTA | 5567 5568 | N CA | SER H 112 SER H 112 | 2 | 4.564 | | 12.424 | 1.0 | 0 62.06 | | H | C |
| | MOTA MOTA | 5569 | CB | SER H 112 | | 5.076 | | | _ | 0 62.27 0 63.44 | | H H | C |
| | MOTA | 5570 | OG | SER H 112 SER H 112 | | 4.805 3.061 | | | 1.0 | 0 64.01 | | H | С |
| 55 | ATOM ATOM | 5571 5572 | C O | SER H 112 SER H 112 | | 2.269 | 64.096 | 11.871 | 1.0 | 0 64.87 | | H H | N O |
| 33 | MOTA | 5573 | N | ALA H 113 | | 2.634 | | | _ | 00 65.89 00 67.77 | | H | C |
| | MOTA | 5574 | | ALA H 113 ALA H 113 | | 1.219 | | 15.179 | 1.0 | 00 67.00 | | H | C |
| | MOTA MOTA | | | ALA H 113 | 2 | 0.861 | L 67.04 | 3 12.965 | | 00 69.23 | | H H | C 0 |
| 60 | MOTA | 5577 | 0 | ALA H 113 | | .9.729 21.836 | | | | 00 69.99 | | H | N |
| | MOTA | | | ALA H 114 ALA H 114 | | 1.55 | | 5 11.383 | 3 1.0 | 00 71.20 | | H | C |
| | MOTA MOTA | | | ALA H 114 | 2 | 22.83 | 2 69.47 | | | 00 70.37 00 72.68 | | H H | C |
| | MOTA | 5581 | | ALA H 114 ALA H 114 | | 20.864 20.69 | | | 7 1. | 00 72.43 | | H | 0 |
| 65 | ATOM ATOM | | | LYS H 115 | | 20.52 | 3 69.29 | 3 9.30 | 7 1. | 00 73.47 | | H H | C N |
| | MOTA | 5584 | L CA | LYS H 115 | | 19.58 18.33 | | | | 00 74.97 00 76.29 | | Н | С |
| | MOTA | | | LYS H 115 LYS H 115 | | 17.02 | | | | 00 78.90 | | H | С |
| | MOTA | , ,,,,,,, | , | | | 250 | | | | | | | |

| | | **** | | | | | | | | | _ | ~ |
|----|---|--------------|-----------|------------------------|------------------|-------------|------------------|--------------------|-------|----------------------|--------|--------------|
| | MOTA | 5587 | | YS H 115 | 15.72 14.47 | | 70.076 59.941 | 8.445 9.414 | 1.00 | 80.84 82.54 | H H | C C |
| | | | CE L | YS H 115 YS H 115 | 13.41 | 7 7 | 70.968 | 9.050 | 1.00 | 84.38 74.57 | H H | C N |
| | MOTA | 5590 | C P | YS H 115 YS H 115 | 20.23 20.97 | - | 69.344 70.400 | 6.901 6.712 | 1.00 | 74.15 | H | 0 |
| 5 | | | | HR H 116 | 19.76 | 1 (| 68.565 | 5.925 | | 74.05 74.84 | H H | N C |
| | ATOM | 5593 | CA T | HR H 116 | 20.33 20.18 | | 68.731 67.575 | 4.659 3.700 | 1.00 | 75.81 | H | C |
| | MOTA | 5594 5595 | CB T | HR H 116 HR H 116 | 19.39 | | 67.962 | 2.580 | 1.00 | 78.72 | H | 0 |
| 10 | ATOM ATOM | 5596 | CG2 T | HR H 116 | 19.52 | 0 | 66.458 | 4.332 4.138 | | 77.18 74.35 | H H | C C |
| 10 | MOTA | | | THR H 116 THR H 116 | $20.04 \\ 19.01$ | | 70.095 70.595 | 4.371 | 1.00 | 74.89 | H | 0 |
| | ATOM ATOM | 5598 5599 | N T | THR H 117 | 21.02 | 8 | 70.736 | 3.524 | 1.00 | 73.19 72.52 | H H | N C |
| | ATOM | 5600 | CA T | THR H 117 | 20.73 21.32 | | 72.009 73.135 | 2.879 3.718 | 1.00 | 72.50 | H | C |
| 15 | MOTA MOTA | 5601 5602 | CB T | ГНК Н 117 ГНК Н 117 | 21.00 | 9 | 72.949 | 5.153 | | 72.65 | H H | O C |
| | ATOM | 5603 | CG2 | THR H 117 | 20.67 | - | 74.469 72.133 | 3.161 1.516 | 1.00 | 71.32 71.62 | n H | C |
| | MOTA | 5604 | C | THR H 117 THR H 117 | 21.30 22.44 | - | 71.904 | 1.379 | 1.00 | 72.24 | H | 0 |
| 20 | MOTA ATOM | 5605 5606 | N] | PRO H 118 | 20.55 | 8 | 72.464 | 0.497 | | 70.54 70.30 | H H | C N |
| 20 | MOTA | 5607 | CD 1 | PRO H 118 | 19.10 21.1 | | 72.729 72.613 | 0.435 -0.815 | 1.00 | 69.81 | H | С |
| | ATOM ATOM | 5608 5609 | CA I | PRO H 118 PRO H 118 | 19.9 | | 72.676 | -1.794 | 1.00 | 70.03 | H H | C |
| | ATOM | 5610 | CG : | PRO H 118 | 18.90 | | 73.314 73.820 | -1.007 -0.850 | 1.00 | 69.36 69.30 | H | Č |
| 25 | ATOM | 5611 5612 | 0 | PRO H 118 PRO H 118 | 22.00 22.1 | 00 | 74.702 | -0.001 | 1.00 | 68.93 | H | O |
| | MOTA MOTA | 5613 | N | PRO H 119 | 23.0 | 20 | 73.759 | -1.772 -2.675 | 1.00 | 69.63 69.24 | H H | N C |
| | MOTA | 5614 | | PRO H 119 PRO H 119 | 23.3 23.9 | | 72.607 74.865 | -1.927 | 1.00 | 69.43 | H | C |
| 30 | ATOM ATOM | 5615 5616 | | PRO H 119 | 25.1 | 40 | 74.229 | -2.653 | 1.00 | 69.59 69.96 | H H | C |
| 30 | MOTA | 5617 | CG | PRO H 119 | 24.4 23.3 | | 73.207 75.894 | -3.526 -2.789 | 1.00 | 69.54 | H | С |
| | MOTA | 5618 5619 | C O | PRO H 119 PRO H 119 | 22.5 | | 75.533 | -3.519 | 1.00 | 69.35 | H | N |
| | MOTA MOTA | 5620 | И | SER H 120 | 23.7 | 35 | 77.137 78.148 | -2.578 -3.511 | | 69.05 69.34 | H H | C |
| 35 | MOTA | 5621 | CA CB | SER H 120 SER H 120 | 23.5 23.3 | | 79.438 | -2.776 | 1.00 | 69.06 | H | C |
| | $\begin{array}{c} \texttt{MOTA} \\ \texttt{ATOM} \end{array}$ | 5622 5623 | OG | SER H 120 | 22.2 | 80 | 79.351 | -1.990 -4.362 | 1.00 | 0 69.83 0 69.65 | H H | О С |
| | ATOM | 5624 | C | SER H 120 | 24.7 25.8 | | 78.222 78.200 | -4.302 -3.817 | 1.00 | 0 70.99 | H | 0 |
| 40 | MOTA MOTA | 5625 5626 | N | SER H 120 VAL H 121 | 24.6 | 83 | 78.406 | -5.682 | 1.00 | 0 69.07 0 68.49 | H H | N C |
| 40 | MOTA | 5627 | CA | VAL H 121 | 25.7 25.5 | | 78.429 77.269 | -6.568 -7.538 | 1.0 | 0 67.99 | H | C |
| | MOTA | 5628 5629 | CB CG1 | VAL H 121 VAL H 121 | 26.6 | | 77.227 | -8.681 | 1.0 | 0 66.50 | H | C |
| | ATOM ATOM | 5630 | CG2 | VAL H 121 | 25.5 | | 75.933 79.759 | -6.683 -7.337 | 1.0 | 0 67.19 0 68.59 | H H | C |
| 45 | ATOM | 5631 | C O | VAL H 121 VAL H 121 | 25.9 25.0 | | 80.213 | -7.833 | 1.0 | 0 69.44 | H | O |
| | MOTA MOTA | 5632 5633 | И | TYR H 122 | 27.0 | 35 | 80.351 | -7.514 | | 0 68.04 0 68.49 | H H | C N |
| | MOTA | 5634 | | TYR H 122 TYR H 122 | 27.0 27.3 | | 81.683 82.741 | -8.072 -7.030 | 1.0 | 0 66.91 | H | С |
| 50 | MOTA MOTA | 5635 5636 | | TYR H 122 | 26. | 318 | 82.787 | -5.901 | 1.0 | 0 65.94 0 65.72 | H H | C |
| 50 | MOTA | 5637 | CD1 | TYR H 122 | 25. 24. | | 82.941 82.968 | -6.191 -5.212 | | 0 64.55 | H | С |
| | MOTA ATOM | 5638 5639 | | | 26. | | 82.585 | -4.584 | 1.0 | 0 64.79 | H H | C |
| | ATOM | 5640 | _ | TYR H 122 | 25. | | 82.631 82.849 | -3.591 -3.962 | | 00 64.05 00 63.93 | H | Č |
| 55 | MOTA | 5641 | | TYR H 122 TYR H 122 | 24. 23. | | 82.929 | -3.129 | 1.0 | 0 63.03 | H | 0 |
| | MOTA MOTA | 5642 5643 | | TYR H 122 | 28. | 278 | 81.724 | -9.056 | | 00 69.84 00 69.11 | H H | C |
| | MOTA | 5644 | l O | TYR H 122 | | 303 142 | | -8.764 -10.181 | 1.0 | 00 71.60 | H | N |
| 60 | MOTA MOTA | 5645 5646 | | PRO H 123 PRO H 123 | | 999 | 83.253 | -10.618 | 3 1.0 | 00 71.61 | H H | C |
| 60 | ATOM | 5647 | 7 CA | PRO H 123 | | 225 | | -11.168 -12.519 | | 73.00 72.20 | H | С |
| | MOTA | 5648 | | PRO H 123 PRO H 123 | | 495 297 | 83.644 | -12.07 | 7 1.0 | 00 71.53 | H | C |
| | ATOM ATOM | | | PRO H 123 | 30. | 228 | 83.455 | -10.82 | 9 1.0 | 00 74.28 00 75.03 | H H | C O |
| 65 | MOTA | 5653 | 1 0 | PRO H 123 LEU H 124 | | 839 500 | | -10.39 | 7 1. | 00 75.57 | H | \mathbf{N} |
| | MOTA MOTA | | | LEU H 124 | 32 | 464 | 84.215 | -10.80 | 8 1. | 00 77.18 | H H | C |
| | ATOM | 565 | 4 CB | LEU H 124 | | 515 | | | | 00 76.33 00 75.63 | H | c |
| | MOTA | 565 | 5 CG | LEU H 124 | | . 045 50 | , 05.17 | J | · | | | |
| | | | | | | 44 F | | | | | | |

| | ATOM ATOM ATOM | 5657 | CD2 C | LEU H 124 LEU H 124 LEU H 124 LEU H 124 | 32.585 | | -7.902 -7.676 -12.061 -12.645 | 1.00 7 1.00 7 | 5.22 8.64 8.81 | H H H | Ŧ | 0000 |
|----|--------------------------------------|--------------------------------------|----------------------------|---|--|--|---|--------------------------------------|---|-------------|-----------------------|------------------|
| 5 | ATOM ATOM ATOM ATOM ATOM | 5660 5661 5662 5663 | N CA | ALA H 125 ALA H 125 ALA H 125 ALA H 125 | 33.005 33.442 32.252 34.258 | 85.915 86.473 86.765 87.705 | -12.348 -13.631 -14.462 -13.366 | 1.00 8 | 2.49 1.49 3.38 | I I I | H H H H H | И С С |
| 10 | MOTA ATOM ATOM MOTA | 5664 5665 5666 5667 | O N CD CA | ALA H 125 PRO H 126 PRO H 126 PRO H 126 | 33.977 35.298 35.713 36.216 37.083 | 87.967 87.225 89.095 | -12.373 -14.181 -15.370 -13.959 -15.205 | 1.00 8 | 4.62 4.56 5.66 |]]] | H H H H | C C |
| 15 | ATOM ATOM ATOM | 5668 5669 5670 | CB CG C | PRO H 126 PRO H 126 PRO H 126 | 36.296 35.534 | 88.308 90.465 90.903 | -16.113 -13.871 | 1.00 8 | 4.85 | ! | H H H | C C |
| | ATOM ATOM ATOM | 5671 5672 5673 | O N CA | PRO H 126 ALA H 133 ALA H 133 | 34.537 45.015 46.014 | 88.620 88.473 | -19.518 -20.570 -19.927 | 1.00 8 | 37.90 38.86 | | H H H | N C C |
| 20 | ATOM ATOM ATOM ATOM ATOM | 5674 5675 5676 5677 5678 | CB O N CA | ALA H 133 ALA H 133 ALA H 133 ALA H 134 ALA H 134 | 47.399 45.850 44.766 46.979 46.941 | 87.150 86.594 86.669 85.423 | -21.322 -21.442 -21.875 -22.633 | 1.00 8 1.00 8 1.00 8 | 39.28 39.70 39.69 90.00 | | H H H H H | C N C C |
| 25 | ATOM ATOM ATOM ATOM | 5679 5680 5681 5682 | CB C O N | ALA H 134 ALA H 134 ALA H 134 MET H 135 | 48.337 45.920 45.215 45.887 | 84.439 83.736 84.376 | -22.766 -20.712 | 1.00 9 1.00 9 1.00 9 1.00 9 | 90.19 90.05 89.65 | | H H H H | 0 0 0 |
| 30 | MOTA ATOM ATOM ATOM ATOM ATOM | 5683 5684 5685 5686 5687 | CA CB CG SD CE | MET H 135 MET H 135 MET H 135 MET H 135 MET H 135 | 44.974 45.807 46.718 45.790 44.934 | 82.459 81.595 80.601 79.553 | -20.115 -21.291 -20.106 | 1.00 1.00 1.00 | 89.05 89.97 92.18 90.49 | | Н Н Н Н | C C S C |
| 35 | ATOM ATOM ATOM ATOM | 5688 5689 5690 5691 | C O N CA | MET H 135 MET H 135 VAL H 136 VAL H 136 | 43.977 44.172 42.854 41.838 40.793 | 84.167 85.301 83.477 84.065 84.742 | -18.736 -18.881 -18.018 | 1.00 1.00 1.00 1.00 | 87.12 85.50 83.76 | | H H H H H | C N C C |
| 40 | ATOM ATOM ATOM ATOM | 5692 5693 5694 5695 | CB CG1 CG2 C | | 39.802 40.041 41.164 40.857 | 83.703 85.793 83.009 | -19.426 | 1.00 1.00 1.00 1.00 | 83.33 83.66 82.18 82.47 | | Н Н Н Н | 0 0 0 0 |
| | ATOM ATOM ATOM ATOM | 5696 5697 5698 5699 | N CA CB | THR H 137 THR H 137 THR H 137 | 40.974 40.306 41.222 40.560 | 83.371 82.454 82.227 82.675 | L -15.858 1 -14.943 7 -13.740 | $\frac{1.00}{1.00}$ | 80.41 79.76 79.32 79.45 | | H H H H | И С О |
| 45 | MOTA MOTA MOTA | 5700 5701 5702 5703 | OG: CG: O | 2 THR H 137 THR H 137 THR H 137 | 42.519 38.957 38.773 | 83.023 83.013 84.213 | | 1.00 1.00 1.00 | 78.61 78.49 78.29 77.73 | | H H H H | 0 C C |
| 50 | MOTA MOTA MOTA | 5704 5705 5706 5707 | CA CB CG | LEU H 138 LEU H 138 | 38.056 36.717 35.784 36.149 | 82.19 81.76 82.43 | 6 -13.866 8 -14.997 1 -16.321 | 1.00 1.00 1.00 | 77.47 78.10 79.50 79.35 | | H H H H | 000 |
| 55 | ATOM ATOM ATOM ATOM ATOM | 5708 5709 5710 5711 5712 | CD C | 1 LEU H 138 2 LEU H 138 LEU H 138 LEU H 138 GLY H 139 | 35.422 35.787 36.566 37.440 35.428 | 83.91 81.21 80.40 81.31 | 0 -17.526 7 -16.316 7 -12.706 2 -12.420 8 -11.999 | 1.00 1.00 1.00 1.00 | 78.82 76.73 76.08 76.19 | | н н н н | О О С |
| 60 | MOTA MOTA MOTA MOTA | 5713 5714 5715 5716 | CA C O N | GLY H 139 GLY H 139 GLY H 139 CYS H 140 | 35.185 33.699 32.807 33.460 32.115 | 80.19 80.74 79.32 | 3 - 9.639 | 1.00 1.00 1.00 1.00 1.00 | 76.09 75.94 75.89 76.35 76.80 | | H H H H | C O N C |
| 65 | MOTA MOTA MOTA MOTA MOTA | 5718 5719 5720 5721 | 3 C 9 O 0 CE L SG | CYS H 140 CYS H 140 3 CYS H 140 5 CYS H 140 | 32.118 32.979 31.768 30.531 31.166 | 78.99 78.40 77.60 77.71 | 00 -7.062 08 -9.693 6 -10.993 75 -7.033 | 2 1.00 3 1.00 3 1.00 3 1.00 | 75.34 75.52 78.19 83.30 73.47 | | H H H H | C O C S N |
| | MOTA MOTA MOTA | 5723 | 3 C <i>F</i> | A LEU H 141 | 31.133 31.073 | 79.58 | 30 -5.59 | 9 1.00 2 1.00 | 70.98 70.21 | | H | C |

| | ** | | | 30.910 | 81.245 | -3.583 1 | 1.00 69.27 | Н | С |
|----|--------------|----------------------|-----------------------------|------------------|----------------------|------------------|--------------------------|--------|--------|
| | MOTA MOTA | 5726 CD1 | LEU H 141 LEU H 141 | 32.100 | 80.826 | -2.720 | 1.00 68.13 1.00 68.78 | H H | C C |
| | MOTA | 5727 CD2 | LEU H 141 LEU H 141 | | 78.722 | -5.186 | 1.00 69.23 | H | С |
| 5 | MOTA MOTA | 5729 O | LEU H 141 | 28.813 30.252 | , | -5.720 -4.287 | 1.00 69.90 1.00 66.68 | H H | N O |
| | ATOM ATOM | 5731 CA | VAL H 142 VAL H 142 | 29.214 | 76.863 | -3.806 | 1.00 64.25 1.00 64.24 | H H | C |
| | ATOM | 5732 CB | VAL H 142 VAL H 142 | 29.617 28.544 | 75.452 74.440 | -3.846 | 1.00 61.94 | H | C |
| 10 | ATOM ATOM | 5733 CG1 5734 CG2 | VAL H 142 | 29.797 | 75.400 77.012 | -5.719 -2.312 | 1.00 61.98 1.00 63.46 | H H | C C |
| | ATOM ATOM | 5735 C 5736 O | VAL H 142 VAL H 142 | 29.063 29.931 | 76.683 | -1.511 | 1.00 62.73 | H H | O N |
| | ATOM | 5737 N | LYS H 143 | 27.895 27.728 | 77.604 78.239 | -0.671 | 1.00 62.44 1.00 61.55 | H | С |
| 15 | ATOM ATOM | 5738 CA 5739 CB | LYS H 143 LYS H 143 | 27.568 | 79.740 | -0.912 0.368 | 1.00 61.63 1.00 64.18 | H H | C |
| ,0 | ATOM | 5740 CG 5741 CD | LYS H 143 LYS H 143 | 27.800 27.452 | 80.536 82.004 | 0.237 | 1.00 66.95 | Н | С |
| | MOTA MOTA | 5742 CE | LYS H 143 | 27.476 28.805 | 82.690 82.543 | $1.597 \\ 2.222$ | 1.00 67.20 1.00 69.98 | H H | C N |
| 20 | ATOM ATOM | 5743 NZ 5744 C | LYS H 143 LYS H 143 | 26.502 | 77.737 | 0.069 | 1.00 60.08 1.00 59.81 | H H | C O |
| 20 | ATOM | 5745 O | LYS H 143 GLY H 144 | 25.390 26.809 | 77.671 77.297 | -0.439 1.302 | 1.00 58.65 | Н | N |
| | MOTA ATOM | 5746 N 5747 CA | GLY H 144 GLY H 144 | 25.785 | 77.102 | 2.318 2.273 | 1.00 58.01 1.00 57.98 | H H | C |
| | MOTA | 5748 C 5749 O | GLY H 144 GLY H 144 | 25.114 23.925 | 75.718 75.575 | 2.485 | 1.00 57.35 | H | 0 |
| 25 | MOTA MOTA | 5750 N | TYR H 145 | 25.914 25.310 | 74.670 73.332 | 1.969 1.814 | 1.00 57.90 1.00 57.33 | H H | N C |
| | ATOM ATOM | 5751 CA 5752 CB | TYR H 145 TYR H 145 | 25.754 | 72.732 | 0.470 | 1.00 57.61 1.00 59.84 | H H | C C |
| | MOTA | 5753 CG | TYR H 145 | 27.211 27.702 | 72.419 71.225 | 0.469 0.973 | 1.00 59.62 | H | С |
| 30 | MOTA MOTA | 5754 CD1 5755 CE1 | 1 TYR H 145 | 29.021 | 70.862 | 0.786 -0.241 | 1.00 61.69 1.00 60.20 | H H | C |
| | MOTA | 5756 CD2 5757 CE2 | | 28.071 29.408 | 73.235 72.879 | -0.428 | 1.00 60.85 | H | C |
| • | MOTA MOTA | 5758 CZ | TYR H 145 | 29.887 31.233 | 71.699 71.371 | 0.108 -0.008 | 1.00 61.51 1.00 63.36 | H H | 0 |
| 35 | MOTA MOTA | 5759 OH 5760 C | TYR H 145 TYR H 145 | 25.707 | 72.391 | 2.974 | 1.00 57.16 1.00 56.86 | H H | 0 0 |
| | MOTA | 5761 O | TYR H 145 PHE H 146 | 26.691 24.907 | 72.595 71.338 | 3.662 3.216 | 1.00 57.23 | H | N |
| | MOTA MOTA | 5762 N 5763 CA | PHE H 146 | 25.269 | 70.307 | 4.209 5.618 | 1.00 57.03 1.00 57.40 | H H | C |
| 40 | MOTA | 5764 CB 5765 CG | | 24.977 25.239 | 70.863 69.831 | 6.686 | 1.00 57.38 | H | C |
| | ATOM ATOM | 5766 CD | 1 PHE H 146 | 26.497 24.228 | 69.744 68.953 | 7.267 7.079 | 1.00 56.79 1.00 57.31 | H H | C |
| | MOTA MOTA | 5767 CD 5768 CE | 1 PHE H 146 | 26.753 | 68.781 | 8.233 | 1.00 56.84 1.00 57.73 | H H | C |
| 45 | MOTA | 5769 CE | 22 PHE H 146 3 PHE H 146 | 24.492 25.753 | 67.991 67.889 | 8.047 8.614 | 1.00 56.94 | H | C |
| | MOTA MOTA | 5770 CZ 5771 C | PHE H 146 | 24.395 | 69.079 69.177 | 3.936 3.600 | 1.00 57.78 1.00 58.27 | H H | С 0 |
| | MOTA MOTA | 5772 O 5773 N | PHE H 146 PRO H 147 | 23.225 24.948 | 67.837 | 4.033 | 1.00 57.91 | H H | С И |
| 50 | MOTA | 5774 CI | PRO H 147 | 24.299 26.347 | | 3.760 4.399 | 1.00 57.22 1.00 56.51 | H | C |
| | MOTA MOTA | 5775 CA 5776 CE | 3 PRO H 147 | 26.337 | 66.155 | 4.958 | 1.00 57.13 1.00 57.27 | H H | C C |
| | MOTA | 5777 CG | PRO H 147 PRO H 147 | 25.316 27.195 | | 3.130 | 1.00 56.56 | H | С |
| 55 | ATOM ATOM | | PRO H 147 | 26.749 | 67.891 | 2.031 | 1.00 55.45 1.00 55.99 | H H | N O |
| | ATOM | | | 28.481 29.360 | 66.829 | 2.227 | 1.00 55.91 | H H | C |
| | MOTA MOTA | 5782 CI | B GLU H 148 | 30.818 31.483 | | | | H | С |
| 60 | ATOM ATOM | 5784 C | D GLU H 148 | 32.922 | 68.092 | 2.735 | 1.00 60.41 | H H | C 0 |
| 30 | ATOM | 5785 O | E1 GLU H 148 | 33.838 33.11 | 3 67.843 7 68.614 | 3.478 4.641 | 1.00 60.21 | H | 0 |
| | MOTA MOTA | | GLU H 148 | 28.86 | 6 65.468 | 1.672 | | H H | C |
| 65 | ATOM | 5788 O | 110 | 28.27 29.15 | 6 65.243 | 0.375 | 1.00 54.06 | H H | N C |
| 65 | MOTA MOTA | 5790 C | D PRO H 149 | 28.96 29.91 | 5 63.97 | | 1.00 54.94 | H | C |
| | ATON ATON | | A PRO H 149 B PRO H 149 | 30.90 | 9 65.16 | 7 -1.114 | 1.00 54.57 | H H | C |
| | ATOM | • | G PRO H 149 | 30.05 | 7 63.94 | 4 -1.504 | ± 1.00 Jæ.æ2 | ** | _ |
| | | | | 262 | | | | | |

| | μ | | | | 20 121 | 66.781 | -1.643 | 1.00 5 | 6.29 | H | С |
|----|--------------|--------------|------------|------------------------|------------------|------------------|-------------------------|---------------------|--------------------|--------|--------|
| | MOTA | J , J = | | RO H 149 RO H 149 | 29.121 27.930 | 66.563 | -1.847 | 1.00 5 | 7.63 | H | 0 |
| | MOTA MOTA | J. J. | N A | AL H 150 | 29.844 | 67.654 | -2.427 | 1.00 5 | | H H | N C |
| | MOTA | J , J - | CA V | AL H 150 | 29.324 | 68.079 | -3.723 -3.809 | 1.00 5 | | H | Č |
| 5 | MOTA | J.J. | CB V | AL H 150 | 29.146 28.016 | 69.608 70.105 | -2.912 | 1.00 5 | 55.69 | H | C |
| | MOTA | • | CG1 V | AL H 150 AL H 150 | 30.449 | 70.326 | -3.507 | 1.00 5 | | H | C |
| | MOTA MOTA | 5000 | C V | AL H 150 | 30.290 | 67.734 | -4.807 | 1.00 5 | | H H | С О |
| | ATOM | 00- | O V | AL H 150 | 31.430 | 67.338 67.938 | -4.587 -6.018 | | 59.16 | H | N |
| 10 | MOTA | 5000 | | HR H 151 HR H 151 | 29.837 30.715 | 67.629 | -7.095 | 1.00 | 50.28 | H | C |
| | ATOM | | CA T | HR H 151 HR H 151 | 30.353 | 66.211 | -7.573 | 1.00 | 61.13 | H | C |
| | MOTA MOTA | 5805 5806 | OG1 T | HR H 151 | 31.476 | 65.613 | -8.226 | 1.00 | 62.65 61 40 | H H | С О |
| | ATOM | 5807 | - | HR H 151 | 29.132 | 66.233 68.695 | -8.489 -8.174 | | 60.42 | H | č |
| 15 | MOTA | 5808 | | HR H 151 | 30.628 29.556 | 69.171 | -8.551 | 1.00 | 61.43 | H | 0 |
| | MOTA | 5809 5810 | O T | HR H 151 AL H 152 | 31.823 | 69.130 | -8.609 | 1.00 | 60.63 | H | N |
| | MOTA MOTA | 5810 | CA V | AL H 152 | 31.903 | 70.227 | -9.539 | $\frac{1.00}{1.00}$ | 60.80 | H H | C |
| | MOTA | 5812 | CB V | 7AL H 152 | 32.737 | 71.304 72.431 | -8.867 -9.854 | 1.00 | 59.55 | H | С |
| 20 | MOTA | 5813 | CG1 V | 7AL H 152 | 33.050 32.020 | 71.839 | -7.646 | 1.00 | 60.63 | H | С |
| | MOTA | 5814 | CG2 V | /AL H 152 /AL H 152 | 32.626 | 69.789 | -10.789 | 1.00 | | H | C |
| | MOTA MOTA | 5815 5816 | 7 0 | /AL H 152 | 33.667 | 69.158 | -10.717 | | 61.61 63.13 | H H | N O |
| | MOTA | 5817 | и а | THR H 153 | 32.010 | | -11.955 -13.195 | | 64.55 | H | Ĉ |
| 25 | MOTA | 5818 | CA 7 | THR H 153 THR H 153 | 32.739 32.109 | | | 1.00 | 64.46 | H | C |
| | MOTA | 5819 5820 | CB 5 | THR H 153 | 30.720 | | -14.214 | 1.00 | 66.15 | H | O C |
| | MOTA MOTA | 5821 | CG2 | THR H 153 | 32.260 | | | $1.00 \\ 1.00$ | 63.21 65.35 | H H | C |
| | ATOM | 5822 | C : | THR H 153 | 32.639 | | | 1.00 | 65.82 | H | Ö |
| 30 | MOTA | 5823 | 0 ' | THR H 153 TRP H 154 | 31.845 33.50 | 71.320 | -15.015 | 1.00 | 67.73 | H | N |
| | MOTA | 5824 5825 | CA ' | TRP H 154 | 33.34 | 72.395 | 5 -15.980 | | 70.47 | H | C C |
| | MOTA MOTA | 5826 | CB ' | TRP H 154 | 34.61 | 73.250 | -15.939 | 1.00 | 71.18 71.96 | H H | G |
| | MOTA | 5827 | CG | TRP H 154 | 34.74 | |) -14.636) -14.369 | 1.00 | 72.27 | H | С |
| 35 | MOTA | 5828 | | TRP H 154 TRP H 154 | 34.19 34.61 | | -13.034 | 1.00 | 72.93 | H | C |
| | MOTA | 5829 5830 | CE2 CE3 | TRP H 154 | 33.42 | | 2 -15.096 | | 72.34 | H | C |
| | MOTA MOTA | 5831 | CD1 | TRP H 154 | 35.49 | | | 1.00 | 72.81 72.55 | H H | И |
| | MOTA | 5832 | NE1 | TRP H 154 | 35.44 34.23 | | | | | H | С |
| 40 | MOTA | 5833 | CZ2 | TRP H 154 TRP H 154 | 33.05 | | | 1.00 | 73.01 | H | C |
| | MOTA MOTA | 5834 5835 | CZ3 CH2 | TRP H 154 | 33.45 | 3 77.75 | 7 -13.283 | | 73.60 | H H | C |
| | ATOM | 5836 | C | TRP H 154 | 33.10 | | 9 -17.383 0 -17.717 | | 71.96 72.49 | H | ŏ |
| | MOTA | 5837 | 0 | TRP H 154 | 33.63 32.26 | | $\frac{0}{4}$ -18.176 | 1.00 | 73.41 | H | N |
| 45 | ATOM | 5838 | N CA | ASN H 155 ASN H 155 | 31.58 | 5 72.00 | 7 -19.404 | 1.00 | 74.78 | H | C |
| | MOTA | 5839 5840 | CB | ASN H 155 | 32.34 | 4 72.40 | 5 - 20.678 | 3 1.00 | 73.67 | H H | C C |
| | MOTA MOTA | 5841 | CG | ASN H 155 | 32.37 | | 3 -20.835 4 -20.572 | | 72.85 72.15 | H | ŏ |
| | MOTA | 5842 | | ASN H 155 | 31.39 33.58 | | $\frac{4}{3}$ -20.372 | 1 1.00 | 73.17 | H | N |
| 50 | MOTA | 5843 5844 | | ASN H 155 ASN H 155 | 31.21 | 6 70.50 | 2 - 19.442 | 2 1.00 | 76.03 | H | C |
| | MOTA MOTA | | | ASN H 155 | 31.40 | 69.81 | .8 -20.45 | | 76.90 77.24 | H H | И |
| | MOTA | | | SER H 156 | 30.66 | | .0 -18.30 4 -18.23 | | 78.92 | H | C |
| | MOTA | | | SER H 156 | 30.03 28.8 | | 0 -19.22 | 1 1.00 | 79.62 | H | C |
| 55 | MOTA | | | SER H 156 SER H 156 | 27.8 | 7 69.58 | 36 -18.82 | 2 1.00 | 80.28 | H | 0 |
| | MOTA MOTA | | | SER H 156 | 31.0 | L6 67.49 | 1 -18.35 | | 79.81 80.45 | H H | O C |
| | MOTA | | | SER H 156 | 30.6 | | 13 -18.63 28 -18.09 | | 80.43 | H | N |
| | ATOM | | | GLY H 157 | 32.2 33.3 | | 48 -18.14 | 0 1.00 | 0 80.31 | Н | C |
| 60 | ATOM | | | GLY H 157 GLY H 157 | 34.4 | 37 67.34 | 49 -19.03 | 3 1.00 | 0 80.50 | H | C |
| | MOTA MOTA | | | GLY H 157 | 35.6 | 42 66.95 | 51 -18.92 | 3 1.00 | 0 80.73 | H H | N O |
| | ATOM | | | ALA H 158 | 34.0 | | 46 -19.96 | | 0 80.66 0 81.02 | H | C |
| | ATOM | ī 585' | 7 CA | ALA H 158 | 35.0 | | 06 -21.02 33 -22.08 | 9 1.0 | 0 81.05 | H | С |
| 65 | MOTA | ı 5858 | | ALA H 158 ALA H 158 | 34.2 36.3 | 06 69.29 | 92 -20.52 | 5 1.0 | 0 81.09 | H | C |
| | ATOM | | | ALA H 158 | 37.4 | 07 68.84 | 48 -20.78 | 9 1.0 | 0 80.82 | H H | |
| | ATOM ATOM | | | LEU H 159 | 36.1 | 20 70.4 | 02 -19.77 | | 0 81.48 0 81.12 | H H | |
| | MOTA | | | LEU H 159 | 37.2 | | 34 -19.22 | .0 1.0 | 0 01.12 | •• | _ |
| | | | | | 263 | | | | | | |

| | | | | | | 1 | 10 026 | 1.00 81.49 | Н | С |
|-----|--------------|--------------|---------|--------------------------|------------------|----------------------|-------------------|--------------------------|--------|--------------------------|
| | MOTA | | | LEU H 159 | 36.718 | 72.524 - 73.540 - | 18.926 | 1.00 80.68 | H | Č |
| | MOTA | 5864 | CG | LEU H 159 | 37.224 36.514 | 74.885 - | | 1.00 80.53 | н | С |
| | MOTA | | CD1 | LEU H 159 | 38.716 | 73.822 - | 19.816 | 1.00 81.02 | H | C |
| | ATOM | _ | | LEU H 159 LEU H 159 | 37.786 | 70.536 - | 17.917 | 1.00 81.10 | H | С |
| 5 | ATOM | | | LEU H 159 | 37.150 | 70.570 - | 16.885 | 1.00 80.67 | H | 0 |
| | MOTA | - | N O | SER H 160 | 39.002 | 69.969 - | 17.978 | 1.00 81.36 | H | $\widetilde{\mathbf{N}}$ |
| | ATOM ATOM | | CA | SER H 160 | 39.491 | 69.283 - | | 1.00 81.20 | H | C |
| | ATOM | 5871 | CB | SER H 160 | 39.458 | • • • | 17.075 | 1.00 81.88 | H | C |
| 10 | ATOM | 5872 | OG | SER H 160 | 39.477 | | 18.489 | 1.00 82.71 | H H | O C |
| 10 | ATOM | | Ċ | SER H 160 | 40.911 | 69.699 - | -16.408 | 1.00 80.76 1.00 81.69 | H | Ö |
| | MOTA | 5874 | ō | SER H 160 | 41.486 | 69.249 - | -15.415 | 1.00 81.69 | H | N |
| | ATOM | 5875 | N | SER H 161 | 41.515 | 70.530 - | -17.297 | 1.00 79.30 | H | Č |
| | MOTA | 5876 | CA | SER H 161 | 42.797 | 71.127 - | -10.940 17.060 | 1.00 78.13 | H | č |
| 15 | MOTA | 5877 | CB | SER H 161 | 43.864 | 70.721 - 69.356 - | -17.737 | 1.00 80.44 | H | ō |
| | MOTA | 5878 | OG | SER H 161 | 44.212 | | -16.771 | 1.00 76.76 | Н | C |
| | MOTA | 5879 | С | SER H 161 | 42.743 | | -17.292 | 1.00 76.36 | H | 0 |
| | MOTA | 5880 | 0 | SER H 161 | 41.890 | | -15.955 | 1.00 75.51 | H | \mathbf{N} |
| | MOTA | 5881 | N | GLY H 162 | 43.720 | | -15.436 | 1.00 73.39 | H | С |
| 20 | MOTA | 5882 | CA | GLY H 162 | 42.535 | | -14.455 | 1.00 71.72 | H | C |
| | MOTA | 5883 | C | GLY H 162 GLY H 162 | 42.098 | | -14.213 | 1.00 72.43 | H | 0 |
| | MOTA | 5884 | 0 | VAL H 163 | 42.005 | 73.511 | -13.941 | 1.00 68.97 | H | N |
| | MOTA | 5885 5886 | N CA | VAL H 163 | 40.926 | | -12.941 | 1.00 66.41 | H | C |
| 0.5 | MOTA | 5887 | CB | VAL H 163 | 39.906 | 72.375 | -13.308 | 1.00 66.17 | H | C |
| 25 | ATOM ATOM | 5888 | CG1 | VAL H 163 | 39.101 | | -12.064 | 1.00 64.64 | H | C |
| | ATOM | 5889 | CG2 | VAL H 163 | 38.945 | 72.866 | -14.357 | 1.00 65.38 | H H | C |
| | MOTA | 5890 | Ċ | VAL H 163 | 41.427 | 73.170 | -11.526 | 1.00 65.54 1.00 65.66 | Н | ŏ |
| | MOTA | 5891 | 0 | VAL H 163 | 42.045 | | -11.247 | 1.00 65.66 1.00 64.28 | H | Ŋ |
| 30 | ATOM | 5892 | N | HIS H 164 | 41.138 | | -10.634 | 1.00 64.28 | H | Ĉ |
| | ATOM | 5893 | CA | HIS H 164 | 41.380 | 73.986 | -9.217 -8.825 | 1.00 62.70 | H | Č |
| | ATOM | 5894 | CB | HIS H 164 | 42.289 | 75.168 75.002 | -9.366 | 1.00 61.67 | Н | C |
| | MOTA | 5895 | ÇG | HIS H 164 | 43.713 | | -10.192 | 1.00 61.61 | Н | C |
| | MOTA | 5896 | CD2 | HIS H 164 | 44.444 44.548 | 73.994 | -8.998 | 1.00 61.59 | H | N |
| 35 | MOTA | 5897 | ND1 | HIS H 164 | 45.733 | 74.259 | -9.619 | 1.00 61.79 | H | С |
| | MOTA | 5898 | CEI | HIS H 164 HIS H 164 | 45.701 | 75.392 | -10.339 | 1.00 61.73 | H | N |
| | ATOM | 5899 | | HIS H 164 | 40.045 | 74.070 | -8.445 | 1.00 62.25 | H | C |
| | ATOM | 5900 5901 | C | HIS H 164 | 39.417 | 75.114 | -8.357 | 1.00 62.65 | H | 0 |
| 40 | MOTA | 5901 | И | THR H 165 | 39.571 | 72.900 | -7.924 | 1.00 60.50 | H | N |
| 40 | MOTA ATOM | 5902 | CA | THR H 165 | 38.430 | | -6.986 | 1.00 58.57 | H | C |
| | ATOM | 5904 | CB | THR H 165 | 37.531 | 71.679 | -7.383 | 1.00 58.57 | H H | 0 |
| | ATOM | 5905 | OG: | | 36.954 | 71.953 | -8.661 | 1.00 57.87 | п Н | č |
| | MOTA | 5906 | CG: | | 36.394 | | -6.374 | 1.00 56.88 1.00 57.25 | H | č |
| 45 | ATOM | 5907 | С | THR H 165 | 38.921 | | -5.529 -5.164 | 1.00 57.25 | Н | ŏ |
| | ATOM | 5908 | 0 | THR H 165 | 39.631 | | -4.680 | 1.00 55.32 | H | N |
| | MOTA | 5909 | N | PHE H 166 | 38.577 | | -3.346 | 1.00 53.48 | Н | C |
| | MOTA | 5910 | CA | PHE H 166 | 39.188 39.250 | | -2.943 | 1.00 51.93 | H | C |
| | MOTA | 5911 | CB | PHE H 166 | 40.124 | | -3.886 | 1.00 50.87 | н | C |
| 50 | MOTA | 5912 | CG | PHE H 166 1 PHE H 166 | 39.593 | | -5.092 | 1.00 49.87 | H | C |
| | ATOM | 5913 | | 2 PHE H 166 | 41.45 | | -3.551 | 1.00 50.53 | H | |
| | MOTA | 5914 | | 1 PHE H 166 | 40.41 | | -5.980 | 1.00 48.36 | H | |
| | MOTA | 5915 5916 | | | 42.27 | 1 77.110 | -4.445 | 1.00 50.79 | H | C |
| EE | MOTA MOTA | 5917 | | | 41.75 | 2 77.556 | | 1.00 48.16 | H | |
| 55 | ATOM | 5918 | | PHE H 166 | 38.40 | | | | H H | |
| | ATOM | 5919 | | PHE H 166 | 37.21 | | | | | |
| | MOTA | 5920 | | PRO H 167 | 39.13 | | | | | |
| | MOTA | 5921 | | PRO H 167 | 40.55 | | | | | |
| 60 | MOTA | 5922 | | PRO H 167 | 38.46 | | | | | |
| 00 | ATOM | 5923 | | PRO H 167 | 39.56 | | | | | |
| | MOTA | 5924 | r Co | PRO H 167 | 40.87 | | | | Н | |
| | MOTA | 5925 | | PRO H 167 | 37.40 | | | | | |
| | ATOM | 5926 | | PRO H 167 | 37.59 | - | | | | N I |
| 65 | MOTA | | | ALA H 168 | 36.24 35.22 | | | | H | C C |
| | MOTA | | | A ALA H 168 | 33.99 | | |) 1.00 56.59 |) F | |
| | MOTA | | | B ALA H 168 ALA H 168 | 35.72 | | | 1.00 58.43 | } H | |
| | MOTA | | | ALA H 168 | 36.55 | | | | | I 0 |
| | ATOM | 5932 | . 0 | WILL TOO | 264 | | | | | |
| | | | | | 26/ | | | | | |

| | и | | TTDT II 1 CO | 35.216 | 74.412 | 3.348 | 1.00 61.29 | H | N |
|----|--------------|--------------------|--------------------------------|------------------|------------------|------------------|--------------------------|--------|--------|
| | ATOM | 5932 N 5933 CA | VAL H 169 VAL H 169 | | 74.880 | 4.720 | 1.00 64.98 | H | C |
| | ATOM ATOM | 5933 CA 5934 CB | VAL H 169 | 35.947 | 76.274 | | 1.00 65.10 | H H | C |
| | ATOM | 5935 CG1 | L VAL H 169 | | 76.143 | 4.565 | 1.00 64.84 1.00 66.13 | H | C |
| 5 | MOTA | 5936 CG2 | | | 77.109 74.907 | 3.577 5.403 | 1.00 66.34 | H | č |
| - | MOTA | 5937 C | VAL H 169 | 33.945 32.897 | 75.043 | | 1.00 66.63 | H | 0 |
| | MOTA | 5938 O | VAL H 169 LEU H 170 | 33.975 | 74.725 | 6.734 | 1.00 68.77 | H | N |
| | MOTA | 5939 N 5940 CA | LEU H 170 | 32.726 | 74.631 | | 1.00 71.62 | H | C |
| 10 | MOTA MOTA | 5941 CB | LEU H 170 | 32.786 | 73.367 | | 1.00 70.81 1.00 70.04 | H H | C |
| 10 | ATOM | 5942 CG | LEU H 170 | 31.534 | 73.158 | 9.194 8.356 | 1.00 70.04 | H | Č |
| | MOTA | 5943 CD | 1 LEU H 170 | 30.284 | 72.878 71.975 | 10.159 | 1.00 69.05 | H | C |
| | MOTA | | 2 LEU H 170 LEU H 170 | 31.668 32.497 | 75.861 | 8.359 | 1.00 74.42 | Н | C |
| | MOTA | 5945 C 5946 O | LEU H 170 | 33.216 | 76.124 | 9.315 | 1.00 74.98 | H | O |
| 15 | ATOM ATOM | 5947 N | GLU H 171 | 31.473 | 76.650 | 7.985 | 1.00 77.39 | H H | C N |
| | ATOM | 5948 CA | GLU H 171 | 31.147 | 77.829 | 8.780 7.864 | 1.00 80.47 1.00 82.66 | H | Č |
| | MOTA | 5949 CB | GLU H 171 | 31.193 | 79.054 80.220 | 7.804 8.406 | 1.00 85.40 | H | C |
| | MOTA | 5950 CG | | 30.366 31.231 | 81.076 | 9.304 | 1.00 86.56 | H | С |
| 20 | ATOM | 5951 CD 5952 OE | | 30.703 | 81.973 | 9.945 | 1.00 87.03 | H | 0 |
| | ATOM ATOM | 5952 OE | | 32.436 | 80.836 | 9.353 | 1.00 86.28 | H H | С О |
| | ATOM | 5954 C | GLU H 171 | 29.769 | 77.704 | 9.430 | 1.00 81.61 1.00 82.55 | л Н | Ö |
| | ATOM | 5955 O | GLU H 171 | 28.732 | 77.775 77.466 | 8.784 10.755 | 1.00 82.33 | H | N |
| 25 | MOTA | 5956 N | SER H 172 | 29.786 28.538 | 77.280 | 11.487 | 1.00 83.43 | H | С |
| | MOTA | 5957 CA | | 27.828 | 78.630 | 11.604 | 1.00 84.82 | H | C |
| | MOTA | 5958 CE 5959 OG | | 27.626 | 78.930 | 12.985 | 1.00 86.80 | H | 0 |
| | ATOM ATOM | 5960 C | SER H 172 | 27.621 | 76.250 | 10.819 | 1.00 83.32 1.00 83.57 | H H | C O |
| 30 | MOTA | 5961 0 | SER H 172 | 26.564 | 76.556 | 10.283 10.837 | 1.00 83.57 | H | Й |
| | MOTA | 5962 N | ASP H 173 | 28.097 27.315 | 74.987 73.880 | 10.280 | 1.00 80.87 | H | С |
| | MOTA | 5963 CZ | 480 | 27.313 | 72.491 | 10.629 | 1.00 84.20 | H | C |
| | ATOM | 5964 CI 5965 C | 4-0 | 28.158 | 72.411 | 12.114 | 1.00 87.15 | H | C |
| 05 | MOTA MOTA | 5965 CO 5966 OI | D1 ASP H 173 | 28.796 | 73.336 | 12.616 | 1.00 88.19 | H | 0 |
| 35 | ATOM | 5967 O | D2 ASP H 173 | 27.799 | 71.414 | 12.738 | 1.00 88.10 1.00 78.06 | H H | Ċ |
| | ATOM | 5968 C | ASP H 173 | 26.810 | 74.056 73.667 | 8.846 8.487 | 1.00 78.06 1.00 78.01 | H | ŏ |
| | MOTA | 5969 O | 4 🗆 4 | 25.705 27.656 | 74.697 | 8.017 | 1.00 73.95 | H | N |
| | MOTA | 5970 N | 454 | 27.402 | 74.696 | 6.579 | 1.00 70.41 | H | C |
| 40 | MOTA MOTA | 5971 C 5972 C | | 26.488 | 75.875 | 6.219 | 1.00 70.08 | H | C |
| | ATOM | 5973 C | G LEU H 174 | 25.025 | 75.612 | 6.594 | 1.00 70.43 1.00 70.06 | H H | C |
| | MOTA | 5974 C | D1 LEU H 174 | 24.084 | 76.749 | 6.170 5.958 | 1.00 70.00 | H | č |
| | MOTA | | D2 LEU H 174 | 24.469 28.717 | 74.336 74.777 | 5.806 | 1.00 67.79 | Н | С |
| 45 | ATOM | 5976 C | 4 5 4 | 29.660 | 75.460 | 6.187 | 1.00 66.62 | H | 0 |
| | MOTA MOTA | 5977 O 5978 N | | 28.785 | 74.006 | 4.704 | 1.00 64.82 | H | N C |
| | MOTA | | A TYR H 175 | 30.001 | 74.020 | 3.906 | 1.00 62.23 1.00 62.23 | H H | Č |
| | MOTA | | CB TYR H 175 | 30.165 | | 3.264 4.307 | 1.00 62.25 | H | č |
| 50 | MOTA | | CG TYR H 175 | 30.532 31.855 | | 4.721 | 1.00 63.65 | H | C |
| | MOTA | | CD1 TYR H 175 CE1 TYR H 175 | 32.217 | | 5.663 | 1.00 63.25 | H | C |
| | ATOM | | CD2 TYR H 175 | 29.569 | 70.808 | 4.851 | 1.00 62.78 | H | C |
| | ATOM ATOM | | CE2 TYR H 175 | 29.935 | 69.851 | 5.790 | 1.00 63.05 | H H | C |
| 55 | MOTA | | CZ TYR H 175 | 31.254 | | 6.188 7.153 | 1.00 63.80 1.00 65.22 | H | ŏ |
| | MOTA | | OH TYR H 175 | 31.620 29.947 | | 2.834 | 1.00 60.55 | H | C |
| | MOTA | | TYR H 175 | 28.904 | | 2.278 | 1.00 60.47 | H | 0 |
| | ATOM | | O TYR H 175 N THR H 176 | 31.145 | | 2.509 | 1.00 58.14 | H | N |
| | ATOM | | N THR H 176 CA THR H 176 | 31.271 | 76.400 | 1.320 | | H | C |
| 60 | MOTA MOTA | | CB THR H 176 | 31.337 | 77.854 | | | H H | C O |
| | ATOM | | OG1 THR H 176 | 30.080 | 78.266 | | | H | Č |
| | MOTA | 5994 | CG2 THR H 176 | 31.662 | | | | Н | Č |
| | MOTA | 5995 | C THR H 176 | 32.535 33.605 | | | 1.00 54.15 | H | Ο. |
| 65 | ATOM | | O THR H 176 N LEU H 177 | 32.40 | | | 1.00 54.99 | H | И |
| | MOTA | | N LEU H 177 CA LEU H 177 | 33.64 | 4 75.711 | _1.454 | 1.00 54.81 | H | C |
| | MOTA MOTA | | CB LEU H 177 | 33.99 | 7 74.226 | -1.576 | 1.00 53.58 | H H | C |
| | ATOM | | CG LEU H 177 | 33.20 | 5 73.434 | -2.616 | 1.00 53.24 | rı. | C |
| | | | | 265 | | | | | |

| | * CD1 T DI II 177 | 33.308 74.013 -4.022 1.00 51.50 | н С |
|----|--|--|------------|
| | ATOM 6001 CD1 LEU H 177 ATOM 6002 CD2 LEU H 177 | 33.717 71.984 -2.732 1.00 51.97 | н С н С |
| | ATOM 6003 C LEU H 177 | 33.862 70.300 -3.143 1.00 54.75 | н О |
| | ATOM 6004 O LEU H 1// | 34 839 76.548 -3.353 1.00 55.14 | H N H C |
| 5 | AIOH CED U 178 | 34.915 77.210 -4.621 1.00 56.14 | н С н С |
| | ATOM 6007 CB SER H 178 | 35.455 78.055 4 103 1 00 59 10 | н О |
| | ATOM 6008 OG SER H 178 | 35.787 76.403 -5.564 1.00 56.78 | н С н О |
| 40 | ATOM 6010 O SER H 178 | 36.603 75.556 -5.159 1.00 57.21 | H O H N |
| 10 | AHOM 6011 N SER H 179 | 36 339 76 082 -7.932 1.00 58.62 | н С |
| | ATOM 6012 CA SER H 1/9 | 35 518 74 977 -8.584 1.00 58.75 | н С н О |
| | ATOM 6014 OG SER H 179 | 36.313 74.361 -9.613 1.00 59.52 | н О н С |
| 15 | NEOM 6015 C SER H 179 | 35.075 77.125 -9.295 1.00 59.16 | н О |
| | ATOM 6016 O SER H 179 | 37 916 77.008 -9.523 1.00 62.74 | H N H C |
| | AUDM 6018 CA SER H 180 | 38.398 77.958 -10.511 1.00 65.02 | H C |
| | ATOM 6019 CB SER H 180 | 40 701 78 041 -9.914 1.00 65.15 | н О |
| 20 | ATOM 6020 OG SER H 180 | 38 840 77.235 -11.782 1.00 66.68 | н С н О |
| | ATOM 6021 C SER H 180 ATOM 6022 O SER H 180 | 39.221 76.062 -11.807 1.00 66.57 | H O H N |
| | ATOM 6023 N VAL H 181 | 38.720 77.223 14 121 1 00 71 88 | н С |
| | ATOM 6024 CA VAL H 181 | 37 992 76.656 -14.815 1.00 72.40 | н С н С |
| 25 | ATOM 6025 CB VAL H 181 ATOM 6026 CG1 VAL H 181 | 37.011 77.703 -15.337 1.00 71.91 | н С н С |
| | ATOM 6027 CG2 VAL H 181 | 30.409 73.022 25.003 1.00 74.04 | н С |
| | ATOM 6028 C VAL H 181 ATOM 6029 O VAL H 181 | 39.424 79.508 -15.152 1.00 74.01 | H O H N |
| 20 | ATOM 6030 N THR H 182 | 41.088 77.980 -15.536 1.00 76.01 | н С |
| 30 | ATOM 6031 CA THR H 182 | 41.826 78.902 -10.431 -1.00 79.87 | н С |
| | ATOM 6032 CB THR H 182 ATOM 6033 OG1 THR H 182 | 43 322 79.384 -14.540 1.00 80.82 | н О н С |
| | ATOM 6034 CG2 THR H 182 | 43.896 80.294 -16.730 1.00 80.03 | H C |
| 35 | ATOM 6035 C THR H 182 | 41.812 78.403 17.57 1.00 81.90 | н О |
| | ATOM 6036 O THR H 182 | 41.543 79.374 -18.794 1.00 83.41 | H N H C |
| | ATOM 6038 CA VAL H 183 | 41.506 79.122 -20.231 1.00 85.28 | H C |
| | ATOM 6039 CB VAL H 183 | 20.403 77.605 -19.968 1.00 84.54 | H C |
| 40 | ATOM 6040 CG1 VAL H 183 ATOM 6041 CG2 VAL H 183 | 39.201 80.053 -20.320 1.00 84.50 | н С н С |
| | ATOM 6042 C VAL H 183 | 41.963 80.374 -20.976 1.00 86.87 41.665 81.494 -20.600 1.00 86.42 | H O |
| | ATOM 6043 O VAL H 183 | 42 719 80.179 -22.083 1.00 88.54 | H N |
| | ATOM STORY | 43.143 78.934 -22.681 1.00 88.29 | н С н С |
| 45 | ATOM 6046 CA PRO H 184 | 43.109 81.278 24.228 1 00 89 09 | н С |
| | ATOM 6047 CB PRO H 184 | 43.020 79.171 -24.249 1.00 88.32 | н С н С |
| | ATOM 6048 CG PRO H 184 ATOM 6049 C PRO H 184 | 41.942 82.267 -23.160 1.00 90.99 | н С н О |
| 50 | ATOM 6050 O PRO H 184 | 42 265 83 573 -23 196 1.00 92.37 | H N |
| | ATOM 6051 N SER H 185 | 41.175 84.539 -23.307 1.00 93.92 | н С н С |
| | ATTOM 6053 CB SER H 185 | 41.796 85.917 -23.523 1.00 93.71 | н О |
| | ATOM 6054 OG SER H 185 | 40.250 84.197 -24.482 1.00 95.37 | н С |
| 55 | ATOM 6055 C SER H 185 | 39 053 84.030 -24.357 1.00 95.82 | H O H N |
| | ATTOM 6057 N SER H 186 | 40.875 84.129 -25.669 1.00 96.71 | н С |
| | ATTOM 6058 CA SER H 186 | 41 070 92 951 -27 779 1.00 97.22 | H C |
| | ATOM 6059 CB SER H 186 | 42 409 83.051 -27.294 1.00 96.73 | н О Н С |
| 60 | ATOM 6060 OG SER H 186 ATOM 6061 C SER H 186 | 38.872 82.975 -26.564 1.00 98.18 | H C H O |
| | ATTOM 6062 O SER H 186 | 37.732 03.22 | H N |
| | ATOM 6063 N PRO H 187 | 40.347 81.049 -25.882 1.00 99.12 | н С н С |
| 05 | A1011 6365 G7 DPO H 187 | 37.970 80.795 -25.903 1.00 98.81 | H C H C |
| 65 | ATTOM 6066 CB PRO H 187 | 10.050 79.487 -25.685 1.00 99.00 | н С |
| | ATOM 6067 CG PRO H 187 | 36 928 81.342 -24.911 1.00 99.06 | н С н О |
| | ATOM 6068 C PRO H 187 ATOM 6069 O PRO H 187 | 36.101 80.625 -24.368 1.00 99.21 | н О |
| | Alon 0003 0 | 266 | |

| | - | 37.001 82.663 -24.664 1.00 99.35 | н и |
|-----|--|--|------------|
| | ATOM 6070 N ARG H 188 ATOM 6071 CA ARG H 188 | 36.126 83.344 -23.714 1.00 99.40 | н С н С |
| | ATOM 6072 CB ARG H 188 | 36.567 82.959 -22.300 1.00 99.67 35.443 82.305 -21.498 1.00 99.53 | н с |
| _ | ATOM 6073 CG ARG H 188 ATOM 6074 CD ARG H 188 | 34.248 83.247 -21.305 1.00100.06 | H C H N |
| 5 | ATOM 6075 NE ARG H 188 | 33 612 84 726 -19.521 1.00100.11 | н с |
| | ATOM 6076 CZ ARG H 188 ATOM 6077 NH1 ARG H 188 | 32.423 84.150 -19.552 1.00100.16 | H N H N |
| | ATOM 6078 NH2 ARG H 188 | 36 183 84 865 -23.879 1.00 99.18 | н с |
| 10 | ATOM 6079 C ARG H 188 ATOM 6080 O ARG H 188 | 37 230 85.463 -24.085 1.00 99.88 | H O H N |
| | ATOM 6081 N PRO H 189 | 34 695 86 909 -23.868 1.00 98.41 | H C |
| | ATOM 6082 CD PRO H 189 ATOM 6083 CA PRO H 189 | 33.737 84.759 -23.700 1.00 98.37 | н С н С |
| 15 | ATOM 6084 CB PRO H 189 | 32.648 85.752 -23.292 1.00 98.25 33.290 87.128 -23.140 1.00 97.82 | н С |
| | ATOM 6085 CG PRO H 189 ATOM 6086 C PRO H 189 | 33 354 84.074 -25.015 1.00 98.61 | н С н О |
| | ATOM 6087 O PRO H 189 | 32.206 83.732 -25.264 1.00 98.49 34.360 83.922 -25.894 1.00 98.76 | H N |
| | ATOM 6088 N SER H 190 ATOM 6089 CA SER H 190 | 34.104 83.255 -27.163 1.00 98.88 | н С н С |
| 20 | ATOM 6090 CB SER H 190 | 35.433 82.711 -27.684 1.00 99.51 | н С н О |
| | ATOM 6091 OG SER H 190 | 33 098 82.114 -26.993 1.00 98.50 | н С н О |
| | ATOM 6093 O SER H 190 | 31.933 82.211 -27.357 1.00 98.43 | H O H N |
| 25 | ATOM 6094 N GLU H 191 | 32.708 79.880 -26.132 1.00 97.34 | н С н С |
| | ATOM 6096 CB GLU H 191 | 33.438 78.565 -26.415 1.00 98.15 | н С н С |
| | ATOM 6097 CG GLU H 191 | 35.565 77.727 -27.379 1.00100.16 | н С н О |
| 30 | ATOM 6099 OE1 GLU H 191 | 36.435 78.045 -26.581 1.00100.89 | н О Н О |
| 00 | ATOM 6100 OE2 GLU H 191 | 32 264 79.934 -24.669 1.00 96.18 | н С н О |
| | ATTOM 6102 O GLU H 191 | 32.723 80.747 -23.876 1.00 95.98 | H O H N |
| | ATOM 6103 N THR H 192 | 30.724 79.091 -22.994 1.00 93.78 | н С |
| 35 | ATOM 6105 CB THR H 192 | 29.277 78.623 -23.105 1.00 94.05 | н С н О |
| | ATOM 6106 OG1 THR H 192 | 28.440 79.678 -23.840 1.00 93.66 | н С |
| | ATOM 6108 C THR H 192 | 31.487 78.205 -22.002 1.00 92.58 | н С н О |
| 40 | ATOM 6109 O THR H 192 | 31.659 78.811 -20.824 1.00 90.80 | H N |
| | ATOM 6111 CA VAL H 193 | 32.106 78.053 -19.668 1.00 88.60 | н С н С |
| | ATOM 6112 CB VAL H 193 | 33.150 80.273 -19.171 1.00 88.69 | н С |
| 45 | ATOM 6114 CG2 VAL H 193 | 33.506 78.369 -17.610 1.00 87.63 | н С н С |
| 45 | ATOM 6115 C VAL H 193 | 30.403 78.947 -18.214 1.00 87.20 | H O |
| | ATOM 6117 N THR H 194 | 30.587 76.709 -18.396 1.00 85.54 | H N H C |
| | ATOM 6118 CA THR H 194 | 29 370 75 813 -18.285 1.00 83.86 | н С |
| 50 | ATOM 6120 OG1 THR H 194 | 27.816 76.773 -19.185 1.00 84.35 | н О н С |
| | ATOM 6121 CG2 THR H 194 | 29.955 75.585 -16.355 1.00 82.17 | H C |
| | ATOM 6123 O THR H 194 | 30.672 74.613 -16.553 1.00 82.55 | H O |
| 55 | ATOM 6124 N CYS H 195 | 20 051 74 784 -14 145 1.00 78.12 | н С |
| | ATOM 6125 CA CYS H 195 ATOM 6126 C CYS H 195 | 28.846 74.043 -13.572 1.00 76.08 | н С н О |
| | ATOM 6127 O CYS H 195 | 20 925 75 600 -13.095 1.00 79.63 | н С |
| -00 | ATOM 6128 CB CYS H 195 ATOM 6129 SG CYS H 195 | 29 974 75.843 -11.518 1.00 82.89 | н S н N |
| 60 | ATOM 6130 N ASN H 196 | 29.066 72.780 -13.183 1.00 74.40 27.980 71.872 -12.865 1.00 72.95 | н с |
| | ATOM 6131 CA ASN H 196 ATOM 6132 CB ASN H 196 | 27.915 70.606 -13.774 1.00 72.15 | н С н С |
| | ATOM 6133 CG ASN H 196 | 28.406 70.875 -15.164 1.00 71.83 29.525 71 162 -15.381 1.00 68.99 | н О |
| 65 | ATOM 6134 OD1 ASN H 196 ATOM 6135 ND2 ASN H 196 | 27.501 70.826 -16.106 1.00 73.50 | H N H C |
| | ATOM 6136 C ASN H 196 | 28.281 71.399 -11.561 1.00 72.47 | H O |
| | ATOM 6137 O ASN H 196 | 29.217 70.696 -11.342 1.00 72.10 27.318 71.586 -10.735 1.00 71.69 | H N |
| | ATOM 6138 N VAL H 197 | 267 | |

| | " | 6139 | CA | VAL H 1 | 97 | 27.429 | 71.327 | -9.318 | 1.00 | | Н | С |
|------------|--------------|--------------|----------|--------------------|-------|------------------|------------------|------------------------|-------------|--------------------|--------|----------|
| | ATOM ATOM | | | VAL H 1 | | 27.179 | 72.629 | -8.554 | | 69.36 | H | C |
| | ATOM | 6141 | CG1 | VAL H 1 | L97 | 27.229 | 72.357 | -7.046 | 1.00 | 67.95 68.71 | H H | C |
| | ATOM | | | VAL H 1 | | 28.253 | 73.643 70.345 | -9.009 -8.905 | 1 00 | 69.75 | H | C |
| 5 | MOTA | | | VAL H 1 | | 26.381 25.213 | 70.530 | -9.240 | 1.00 | 70.35 | H | Ö |
| | MOTA | 6144 | • | VAL H 1 ALA H 1 | | 26.747 | 69.318 | -8.145 | 1.00 | 68.57 | H | N |
| | MOTA | 6145 6146 | N CA | ALA H | | 25.749 | 68.437 | -7.608 | 1.00 | 67.67 | H | С |
| | MOTA MOTA | 6147 | CB . | ALA H | | 25.841 | 67.205 | -8.296 | 1.00 | 67.30 | H | C |
| 10 | ATOM | 6148 | C | ALA H | 198 | 25.921 | 68.201 | -6.135 | 1.00 | 67.32 | H | C |
| .0 | ATOM | 6149 | 0 | ALA H | 198 | 27.024 | 68.151 | -5.641 | 1.00 | 66.23 67.38 | H H | O N |
| | MOTA | 6150 | N | HIS H | 199 | 24.826 | 67.953 67.804 | -5.469 -4.064 | 1.00 | 68.47 | H | Č |
| | MOTA | 6151 | CA | HIS H | | 24.776 24.255 | 69.073 | -3.271 | 1.00 | 67.96 | H | Č |
| | ATOM | 6152 | CB | HIS H | | 24.233 | 68.894 | -1.791 | 1.00 | 67.23 | H | C |
| 15 | ATOM | 6153 6154 | CD2 | HIS H | | 25.311 | 68.371 | -1.013 | 1.00 | 66.87 | H | C |
| | ATOM ATOM | 6155 | ND1 | HIS H | 199 | 23.282 | 69.150 | -0.952 | 1.00 | 66.44 | H | N |
| | MOTA | 6156 | CE1 | HIS H | 199 | 23.669 | 68.911 | 0.302 | | 67.18 | H H | C N |
| | ATOM | 6157 | NE2 | HIS H | 199 | 24.894 | 68.391 | 0.287 -3.971 | 1.00 1.00 | 66.30 69.13 | H | C |
| 20 | MOTA | 6158 | С | HIS H | 199 | 23.780 | 66.705 67.026 | -3.971 | | 69.67 | H | ŏ |
| | ATOM | 6159 | 0 | HIS H PRO H | 199 | 22.637 24.226 | 65.441 | -4.035 | 1.00 | 69.98 | H | N |
| | MOTA | 6160 6161 | N CD | PRO H | | 25.632 | 65.150 | -4.215 | | 69.33 | H | C |
| | ATOM ATOM | 6162 | CA | PRO H | | 23.392 | 64.222 | -3.910 | 1.00 | 70.75 | H | C |
| 25 | ATOM | 6163 | CB | PRO H | | 24.401 | 63.064 | -3.673 | | 70.87 | H | C |
| | MOTA | 6164 | CG | PRO H | | 25.708 | 63.634 | -4.023 | | 71.25 72.04 | H H | C |
| | ATOM | 6165 | C | PRO H | 200 | 22.503 | 64.261 64.016 | -2.707 -2.771 | 1 00 | 72.64 | Н | ŏ |
| | ATOM | 6166 | 0 | PRO H ALA H | | 21.333 23.032 | 64.644 | -1.571 | 1.00 | | H | N |
| 00 | MOTA | 6167 6168 | N CA | ALA H | 201 | 22.184 | 64.607 | -0.379 | | 72.98 | H | C |
| 30 | MOTA MOTA | 6169 | CB | ALA H | 201 | 22.890 | 65.109 | 0.764 | 1.00 | | H | C |
| | MOTA | 6170 | C | ALA H | 201 | 20.826 | 65.318 | -0.529 | | 73.61 | H H | C O |
| | ATOM | 6171 | 0 | ALA H | 201 | 19.920 | 64.865 | 0.034 | 1.00 | 73.80 74.32 | H | И |
| | MOTA | 6172 | N | SER H | 202 | 20.716 19.446 | 66.390 67.136 | -1.286 -1.396 | 1.00 | 75.64 | H | Ĉ |
| 35 | MOTA | 6173 | CA | SER H SER H | | 19.440 | 68.595 | -0.939 | 1.00 | | H | C |
| | MOTA | 6174 6175 | CB OG | SER H | | 20.291 | 69.315 | -2.024 | 1.00 | | H | 0 |
| | ATOM ATOM | 6176 | C | SER H | | 18.957 | 67.126 | -2.831 | 1.00 | | H | C |
| | ATOM | 6177 | Ö | SER H | 202 | 18.189 | 67.973 | -3.318 | 1.00 | | H H | И |
| 40 | ATOM | 6178 | N | SER H | | 19.464 | | -3.560 -4.827 | 1.00 | | H | C |
| | MOTA | 6179 | CA | SER H | | 18.892 17.413 | 65.969 65.525 | -4.606 | | 77.35 | H | č |
| | ATOM | 6180 | CB | SER H SER H | | 17.284 | | -4.052 | 1.00 | | H | 0 |
| | ATOM ATOM | 6181 6182 | OG C | | | 19.000 | | -5.719 | | 77.79 | H | C |
| 45 | ATOM | 6183 | ŏ | SER H | 203 | 18.065 | | | | 78.13 | H | |
| | ATOM | 6184 | N | THR H | 204 | 20.149 | | | | 77.85 | H H | |
| | ATOM | 6185 | CA | THR H | 204 | 20.306 | | | | 79.06 | H | _ |
| | ATOM | 6186 | CB | THR H L THR H | 204 | 20.920 20.042 | | | | 80.45 | H | |
| F 0 | MOTA | 6187 6188 | CG2 | | | 20.960 | | | 1.00 | 79.18 | H | |
| 50 | MOTA ATOM | 6189 | C | THR H | | 21.192 | | -7.564 | | 79.50 | H | _ |
| | MOTA | 6190 | Ö | THR H | 204 | 22.173 | | | 1.00 | 79.85 | H H | |
| | MOTA | 6191 | N | LYS H | 205 | 20.870 | | | | 80.18 81.64 | H | |
| | MOTA | 6192 | CA | LYS H | 205 | 21.768 21.729 | | -10.481 | | 81.77 | H | |
| 55 | MOTA | 6193 | CB | LYS H LYS H | 205 | 22.428 | | _11.878 | | 83.94 | H | С |
| | ATOM | 6194 6195 | | LYS H | 205 | 23.761 | 68.927 | 7 -12.188 | 1.00 | 85.65 | H | |
| | MOTA MOTA | 6196 | | | 205 | 24.377 | 68.628 | 3 -13.676 | 1.0 | 0 86.61 | H | |
| | ATOM | 6197 | | LYS H | 1 205 | 25.873 | | 2 -13.750 | | 0 87.15 | H | |
| 60 | MOTA | 6198 | | LYS H | 1 205 | 21.510 | | L -10.601 | | 0 82.29 0 82.64 | H H | |
| | MOTA | 6199 | | LYS H | 1 205 | 20.392 | | L -11.148 L -10.571 | | 0 82.71 | H | |
| | ATOM | 6200 | | VAL H | 1 206 | 22.540 22.50 | | $\frac{1}{5}$ -11.125 | | 0 83.11 | H | C |
| | ATOM | 6201 6202 | | | | 22.55 | 74.056 | 5 -10.024 | 1.0 | 0 83.19 | F | |
| 65 | MOTA MOTA | 6202 | | 1 VAL F | | 22.55 | | 0 -10.675 | 5 1.0 | 0 83.85 | H | |
| UU | MOTA | 6204 | . CG | 2 VAL F | 1 206 | 21.38 | 0 73.847 | 7 -9.119 | | 0 82.83 | H H | |
| | ATOM | 6205 | C | VAL I | I 206 | 23.69 | 4 73.338 | $\frac{12.032}{2}$ | | 0 83.70 0 83.58 | F | |
| | ATOM | 6206 | | VAL I | | 24.82 23.42 | | 2 -11.783 4 -13.075 | | 0 84.95 | ŀ | |
| | ATOM | 6207 | N | ASP I | 1 40/ | 23.42 | _ , _ | | | | | |
| | | | | | | | | | | | | |

| | ATOM | 6208 CA ASP H 207 | 24.462 74.532 -14.042 1.00 86.38 24.270 73.858 -15.435 1.00 86.99 | н С н С |
|----|--------------|--|--|------------|
| | MOTA MOTA | 6209 CB ASP H 207 6210 CG ASP H 207 | 24.342 72.302 -15.384 1.00 88.63 | н С н О |
| - | ATOM ATOM | 6211 OD1 ASP H 207 6212 OD2 ASP H 207 | 23.380 71.538 -15.103 1.00 89.52 | H C |
| 5 | MOTA | 6213 C ASP H 207 | 24.456 76.044 -14.123 1.00 87.07 23.501 76.601 -14.580 1.00 86.95 | H O |
| | MOTA MOTA | 6215 N ALA H 208 | 25.484 76.710 -13.580 1.00 87.90 | H N H C |
| | MOTA | 6216 CA ALA H 208 6217 CB ALA H 208 | 25.811 78.899 -12.475 1.00 87.84 | H C |
| 10 | ATOM ATOM | 6218 C ALA H 208 | 26.572 78.528 -14.793 1.00 89.66 | н С н О |
| | MOTA | 6219 O ALA H 208 6220 N LYS H 209 | 25.997 79.265 -15.730 1.00 90.60 | H N H C |
| | ATOM ATOM | 6221 CA LYS H 209 | 26.707 79.881 -16.848 1.00 91.34 25.694 80.141 -17.964 1.00 91.16 | н С |
| 15 | MOTA MOTA | 6222 CB LYS H 209 6223 CG LYS H 209 | 26.283 80.980 -19.098 1.00 91.01 | н С н С |
| | MOTA | 6224 CD LYS H 209 | 25.227 81.362 -20.136 1.00 90.83 25.837 81.992 -21.392 1.00 90.53 | н С |
| | ATOM ATOM | 6225 CE LYS H 209 6226 NZ LYS H 209 | 24.796 82.699 -22.135 1.00 89.44 | H N H C |
| 20 | MOTA | 6227 C LYS H 209 | 26 832 82 071 -15.816 1.00 91.55 | н О |
| | ATOM ATOM | 6229 N ILE H 210 | 28.695 81.276 -16.805 1.00 92.64 | H N H C |
| | MOTA | 6230 CA ILE H 210 6231 CB ILE H 210 | 30.918 82.136 -16.427 1.00 92.09 | н С |
| 25 | MOTA MOTA | 6232 CG2 ILE H 210 | 31.654 83.154 -15.536 1.00 91.71 | H С H С |
| | ATOM | 6233 CG1 ILE H 210 6234 CD1 ILE H 210 | 30.409 80.649 -14.424 1.00 90.25 | н С н С |
| | MOTA MOTA | 6235 C ILE H 210 | 29.192 83.572 -17.570 1.00 95.01 29.623 83.485 -18.713 1.00 95.16 | н С н О |
| 00 | ATOM ATOM | 6236 O ILE H 210 6237 N ALA H 211 | 28.423 84.594 -17.155 1.00 96.52 | H N H C |
| 30 | MOTA | 6238 CA ALA H 211 | 27.957 85.595 -18.107 1.00 97.96 26.989 86.529 -17.376 1.00 97.85 | н С |
| | MOTA MOTA | 6239 CB ALA H 211 6240 C ALA H 211 | 29.105 86.409 -18.708 1.00 99.08 | н С н О |
| | MOTA | 6241 O ALA H 211 | 29 276 87 629 -18.171 1.00100.17 | H N |
| 35 | MOTA MOTA | 6243 CA ALA H 212 | 30.290 88.518 -18.725 1.00101.26 | н С н С |
| | MOTA | 6244 CB ALA H 212 6245 C ALA H 212 | 30.480 89.764 -17.861 1.00101.96 | H C |
| | ATOM ATOM | 6246 O ALA H 212 | 31.345 89.835 -16.998 1.00102.21 | H O H N |
| 40 | MOTA | 6247 N ALA H 213 6248 CA ALA H 213 | 29.750 92.013 -17.360 1.00104.14 | н С |
| | MOTA MOTA | 6249 CB ALA H 213 | 29.407 91.661 -15.911 1.00104.00 31.154 92.615 -17.425 1.00105.06 | H C H C |
| | MOTA MOTA | 6250 C ALA H 213 6251 O ALA H 213 | 31.731 93.023 -16.428 1.00105.39 | н О н О |
| 45 | MOTA | 6252 OXT ALA H 213 | 31.766 92.717 -18.478 1.00105.71 48.040 27.606 -7.533 1.00 43.49 | W O |
| | MOTA MOTA | 6253 O HOH W 1 6254 O HOH W 2 | 56.255 30.910 -4.462 1.00 55.47 | M O M |
| | MOTA | 6255 O HOH W 3 | 26 430 18.335 -11.581 1.00 44.42 | M O |
| 50 | ATOM ATOM | 6257 O HOH W 5 | 35.131 45.610 -13.929 1.00 49.40 | M O |
| | MOTA | 6258 О НОН W 6 | 51.776 59.864 11.192 1.00 42.02 | M O |
| | ATOM ATOM | 6260 O HOH W 8 | 44.767 37.321 -4.124 1.00 42.78 | W O |
| | ATOM | 6261 O HOH W 9 6262 O HOH W 10 | 51.943 57.484 12.566 1.00 39.47 | M O |
| 55 | MOTA MOTA | 6263 O HOH W 11 | 38.747 31.228 -1.651 1.00 43.69 | M 0 |
| | MOTA | | 58.428 47.238 4.389 1.00 48.79 | M 0 |
| | MOTA MOTA | 6266 O HOH W 14 | 43.554 36.444 -2.054 1.00 45.57 57.415 61.701 12.627 1.00 41.49 | W 0 |
| 60 | ATOM | | 61.270 51.287 12.253 1.00 67.52 | W O |
| | MOTA MOTA | 6269 O HOH W 18 | 48.459 41.310 -2.576 1.00 48.81 53.916 29.663 7.818 1.00 48.60 | W O |
| | ATOM ATOM | | 56.558 71.377 -0.532 1.00 48.14 | 0 W |
| 65 | ATOM | 6272 O HOH W 21 | 32.808 27.123 -0.609 1.00 44.93 47.847 62.036 -10.526 1.00 63.97 | M O |
| | MOTA MOTA | 1 6274 O HOH W 23 | 36.925 77.944 -1.838 1.00 50.62 | M O |
| | MOTA | 6275 O HOH W 24 | 26.214 42.194 14.054 1.00 63.38 45.644 56.046 9.966 1.00 42.51 | M O |
| | MOTA | 1 6276 O HOH W 25 | 269 | |

| | 14 | | | | | | | 4 071 | 1.00 72. | 02 | W | 0 |
|------|--------------|--------------|--------|----------|----------|------------------|------------------|---------------------|--------------------|-------|------------|-----|
| | ATOM | 6277 C | | HOH W 2 | | 44.856 | 70.990 | 1.971 | 1.00 72. | 26 | W | Ö |
| | MOTA | 6278 C | | HOH W 2 | | 41.934 | 61.986 | -0.999 -1.348 | 1.00 /0. | | W | ŏ |
| | MOTA | 6279 C |) | HOH W 2 | | 25.281 | 34.502 | -6.980 | 1.00 59 | 50 | W | ŏ |
| | MOTA | |) | HOH W 2 | | 49.892 29.792 | 62.411 66.376 | 5.878 | 1.00 52 | .90 | W | Ö |
| 5 | MOTA | - | 2 | HOH W 3 | | 38.272 | 58.084 | -4.321 | 1.00 65 | .01 | W | Ö |
| | MOTA | | 2 | HOH W 3 | | 27.858 | 55.054 | -6.230 | 1.00 56 | | M | 0 |
| | MOTA | | 2 | HOH W 3 | | 57.799 | 63.672 | -12.243 | 1.00 59 | | M | 0 |
| | MOTA | | 2 | | 4 | 31.795 | 68.789 | 0.185 | 1.00 63 | | M | 0 |
| | MOTA | | 0 | | 5 | 38.425 | 31.427 | -8.589 | | .62 | W | 0 |
| 10 | ATOM | - | 0 | | 6 | 46.860 | 66.957 | -9.197 | 1.00 54 | .26 | M | 0 |
| | ATOM | | 0 | | 7 | 36.028 | 69.393 | -9.044 | 1.00 62 | .22 | M | 0 |
| | ATOM | | 0 | | 8 | 41.452 | 74.029 | 2.581 | 1.00 57 | | M | 0 |
| | ATOM | | 0 0 | | 9 | 61.277 | 8.820 | 8.379 | 1.00 45 | .17 | W | 0 |
| 4 = | ATOM | | 0 | | 10 | 58.226 | 38.911 | 5.165 | 1.00 58 | | W | 0 |
| 15 | ATOM | | 0 | | 11 | 45.000 | 61.694 | 3.280 | 1.00 67 | | W | 0 |
| | MOTA ATOM | | ŏ | | 12 | 32.220 | 33.159 | -1.482 | | .51 | W | 0 |
| | ATOM | | Ö | | 13 | 24.268 | 56.225 | -2.604 | | .87 | W | 0 |
| | ATOM | | ŏ | | 14 | 43.870 | 51.811 | 12.171 | 1.00 43 | | M | 0 |
| 20 | ATOM | | ŏ | | 15 | 45.208 | 48.980 | -4.712 | 1.00 41 | | W | 0 |
| 20 | ATOM | | ŏ | | 16 | 51.086 | 54.354 | -7.830 | 1.00 52 | | W | 0 |
| | ATOM | | ŏ | | 17 | 45.735 | 54.909 | 12.584 | 1.00 47 | | W | 0 |
| | ATOM | | ō | | 48 | 40.670 | 36.691 | -0.514 | 1.00 40 | | W | 0 |
| | ATOM | | 0 | | 49 | 47.855 | 48.291 | -6.195 | 1.00 47 | .98 | W | 0 |
| 25 | ATOM | | 0 | | 50 | 27.975 | 20.736 | -9.226 | 1.00 61 | | W | ő |
| | ATOM | 6302 | 0 | | 51 | 26.649 | 37.011 | 3.912 | 1.00 54 1.00 60 | 26 | W | ŏ |
| | MOTA | 6303 | 0 | | 52 | 40.332 | 12.184 | | 1.00 50 | | W | ŏ |
| | ATOM | 6304 | 0 | | 53 | 26.889 | | | 1.00 42 | | W | ŏ |
| | MOTA | 6305 | 0 | | 54 | 46.332 | 35.286 | | 1.00 47 | 62 | W | ŏ |
| 30 | MOTA | 6306 | 0 | | 55 | 38.286 | 11.976 | | 1.00 74 | . 09 | W | Ö |
| | MOTA | 6307 | Ο, | | 56 | 52.678 | 29.083 49.514 | | 1.00 48 | 8.80 | W | Ö |
| | MOTA | 6308 | 0 | | 57 | 42.010 | 60.323 | | 1.00 51 | . 87 | W | Ō |
| | MOTA | 6309 | 0 | | 58 | 34.530 | 62.030 | | 1.00 67 | 7.89 | W | 0 |
| | MOTA | 6310 | 0 | | 59 | 35.892 32.190 | 8.378 | | 1.00 57 | | W | 0 |
| 35 | MOTA | 6311 | 0 | | 60 | 45.527 | 38.449 | | 1.00 42 | 2.83 | M | 0 |
| | ATOM | 6312 | 0 | | 61 | 45.913 | 56.892 | | 1.00 49 | | W | 0 |
| | MOTA | 6313 | 0 | | 62 | 38.310 | 29.708 | | | 27 | W | 0 |
| | MOTA | 6314 | 0 | | 63 | 54.611 | 60.457 | | 1.00 48 | | W | 0 |
| | ATOM | 6315 | 0 | | 64 65 | 39.898 | | | 1.00 5 | | W | 0 |
| 40 | ATOM | 6316 | 0 | | 66 | 44,938 | | | 1.00 7 | 7.41 | M | 0 |
| | MOTA | 6317 | 0 | | 67 | 22.644 | | | 1.00 78 | 3.49 | W | 0 |
| | MOTA | 6318 | 0 | $HOH\ W$ | 68 | 40.739 | | | 1.00 5 | 7.60 | W | 0 |
| | MOTA | 6319 6320 | 0 | HOH W | 69 | 58.604 | | | 1.00 6 | | M | 0 ' |
| 4 == | MOTA | 6321 | Ö | HOH W | 7Ò | 23.021 | | | 1.00 6 | 4.43 | M | 0 |
| 45 | MOTA MOTA | 6322 | ŏ | HOH W | 72 | 36.562 | | 0.228 | 1.00 5 | | W | 0 |
| | | 6323 | ŏ | HOH W | 73 | 36.156 | 30.941 | | | 4.66 | M | |
| | MOTA MOTA | 6324 | ŏ | HOH W | 74 | 46.575 | | | | 1.03 | M | 0 |
| | ATOM | 6325 | ŏ | HOH W | 75 | 63.106 | 60.743 | | 1.00 6 | 5.63 | W | 0 |
| 50 | MOTA | 6326 | Õ | HOH W | 76 | 27.283 | | | | | W | _ |
| 50 | ATOM | 6327 | O | HOH W | 77 | 42.119 | | | | 9.75 | W | |
| | ATOM | 6328 | 0 | HOH W | 78 | 56.213 | 74.27 | | | 9.07 | W | _ |
| | ATOM | 6329 | 0 | HOH W | 79 | 49.593 | | 4.731 | | T.22 | M. | _ |
| | ATOM | 6330 | 0 | HOH W | 80 | 19.20 | | 6.981 | 1.00 6 | | W W | |
| 55 | ATOM | 6331 | 0 | HOH W | 81 | 62.469 | | | | | ₩. | _ |
| | ATOM | 6332 | 0 | HOH W | 82 | 63.942 | | 9 2.662 | | 2.30 | <i>™</i> | _ |
| | ATOM | 6333 | 0 | HOH W | 83 | 51.559 | | | 1.00 5 | 0 77 | T/s | _ |
| | ATOM | 6334 | 0 | HOH W | 84 | 56.70 | | | | 2 66 | T/s | |
| | ATOM | 6335 | 0 | HOH W | 85 | 56.70 | 3 13.17 | | | | Į∧. | _ |
| 60 | ATOM | 6336 | 0 | HOH W | 86 | 38.70 | | | | | V. • | _ |
| | MOTA | 6337 | 0 | HOH W | 87 | 55.18 | | | | | <i>V</i> , | _ |
| | MOTA | 6338 | 0 | HOH W | 88 | 53.09 | 34.49 | | | | V. | _ |
| | MOTA | 6339 | 0 | HOH W | 89 | 42.57 | | | | ,J.J5 | V | _ |
| | MOTA | 6340 | 0 | HOH W | 90 | 57.34 | | | | | ٧ | _ |
| 65 | MOTA | 6341 | 0 | HOH W | 91 | 61.04 | 5 40.26 | 3 -1.253 | | | V | _ |
| - | MOTA | | 0 | HOH W | 92 | 35.56 | | 1 -15.193 8 4.84 | | | V | _ |
| | MOTA | | 0 | HOH W | 93 | 56.06 | | 9 -10.70 | | | V | |
| | MOTA | | 0 | HOH W | 94 | 42.08 | | | | | | v 0 |
| | MOTA | 6345 | 0 | HOH W | 95 | 30.01 | 1 60.16 | 0.50 | | | • | _ |

| | ATOM 6346 O HOH W 96 ATOM 6347 O HOH W 98 | 8 50.322 24.7/6 -13.192 1.00 51.66 W | |
|----|---|--|-------------|
| 5 | ATOM 6348 O HOH W 99 ATOM 6349 O HOH W 100 ATOM 6350 O HOH W 100 ATOM 6351 O HOH W 100 | 9 58.464 55.474 13.043 1.00 70.56 W O 44.700 36.694 -6.969 1.00 70.56 W O 2 23.656 17.781 -5.182 1.00 68.07 W O 37.411 50.148 -8.219 1.00 52.24 W O 37.411 50.148 -8.219 1.00 66.82 W O | |
| 10 | ATOM 6352 O HOH W 10- ATOM 6353 O HOH W 10- ATOM 6354 O HOH W 10- ATOM 6355 O HOH W 10- ATOM 6356 O HOH W 11- ATOM 6357 O HOH W 11- ATOM 6358 O HOH W 11- | 28.717 35.027 -8.770 1.00 79.00 W O O O O O O O O O O O O O O O O O O | |
| 15 | ATOM 6359 O HOH W 11 ATOM 6360 O HOH W 11 ATOM 6361 O HOH W 11 ATOM 6362 O HOH W 11 ATOM 6363 O HOH W 11 | 14 24.876 23.040 -17.596 1.00 66.24 W O 15 1.643 3.467 3.813 1.00 69.60 W O 16 16 37.627 61.517 4.930 1.00 61.35 W O 17 54.093 37.319 -7.747 1.00 63.69 W O 17 54.093 37.319 -7.747 1.00 63.24 W O | |
| 20 | ATOM 6364 O HOH W 13 ATOM 6365 O HOH W 13 ATOM 6366 O HOH W 13 ATOM 6367 O HOH W 13 | 18 | |
| 25 | ATOM 6369 O HOH W 1: ATOM 6370 O HOH W 1: ATOM 6371 O HOH W 1: ATOM 6372 O HOH W 1 | 23 | |
| 30 | ATOM 6374 O HOH W 1 ATOM 6375 O HOH W 1 ATOM 6376 O HOH W 1 ATOM 6377 O HOH W 1 ATOM 6378 O HOH W 1 | 128 36.172 56.763 14.794 1.00 66.67 W O L30 42.258 8.230 -13.604 1.00 65.20 W O L30 46.138 51.846 16.640 1.00 54.65 W O L31 27.630 60.434 19.677 1.00 59.03 W O L31 27.630 68.255 -15.282 1.00 83.69 W O L32 45.177 68.255 -15.282 1.00 68.39 W O | |
| 35 | ATOM 6379 O HOH W 1 ATOM 6380 O HOH W 1 ATOM 6381 O HOH W 1 ATOM 6382 O HOH W 1 | 133 20.000 32.11 -4.723 1.00 97.13 W O 134 29.093 9.721 -4.723 1.00 97.13 W O 136 51.100 80.703 -12.102 1.00 69.57 W O 137 21.223 52.941 19.573 1.00 89.91 W O 138 39.908 48.609 13.428 1.00 54.77 W O 138 39.908 18.6000 18.6000 18.600 18.600 18.600 18.600 18.600 | |
| 40 | ATOM 6384 O HOH W 3 ATOM 6385 O HOH W 3 ATOM 6386 O HOH W 3 ATOM 6387 O HOH W 3 | $\begin{array}{cccccccccccccccccccccccccccccccccccc$ | |
| 45 | ATOM 6389 O HOH W ATOM 6390 O HOH W ATOM 6391 O HOH W ATOM 6392 O HOH W | 145 |) |
| 50 | ATOM 6394 O HOH W ATOM 6395 O HOH W ATOM 6396 O HOH W ATOM 6397 O HOH W | 150 61.671 43.988 18.926 1.00 73.37 W O 151 53.973 39.898 -6.529 1.00 63.01 W O 152 33.054 13.127 -22.134 1.00 46.54 W O 153 40.317 33.419 9.150 1.00 64.69 W O 153 40.628 68.076 -0.443 1.00 66.41 W |))) |
| 55 | ATOM 6398 O HOH W ATOM 6399 O HOH W ATOM 6400 O HOH W ATOM 6401 O HOH W ATOM 6402 O HOH W ATOM 6403 O HOH W | 154 40.949 12.531 1.841 1.00 57.31 W C C C C C C C C C C C C C C C C C C | |
| 60 | ATOM 6404 O HOH W ATOM 6405 O HOH W ATOM 6406 O HOH W ATOM 6407 O HOH W ATOM 6408 O HOH W | 160 43.374 71.842 8.393 1.00 68.93 W 161 62.463 57.842 8.393 1.00 68.93 W 162 62.314 3.853 -8.007 1.00 72.85 W 163 48.708 28.590 -11.402 1.00 70.46 W 164 26.594 22.894 -11.356 1.00 72.66 W 164 37.650 57.278 -2.348 1.00 75.27 W | 00000 |
| 65 | ATOM 6409 O HOH W ATOM 6410 O HOH W ATOM 6411 O HOH W ATOM 6412 O HOH W ATOM 6413 O HOH W | V 165 27.594 60.020 0.150 1.00 62.76 W V 166 27.594 60.020 0.150 1.00 85.08 W V 167 43.450 54.030 -6.900 1.00 85.08 W V 168 38.122 59.238 -1.849 1.00 56.87 W V 169 27.129 39.301 13.729 1.00 68.09 W V 169 27.129 39.301 50.62 1.00 50.86 W | 00000 |
| | ATOM 6414 O HOH W | 271 | |

| | а | | | | | | | 1 00 55 64 | 7.7 | ^ |
|----|--------------|--------------|---|------------------------|------------------|------------------|------------------------|--------------------------|--------|---|
| | ATOM | 6415 | 0 | HOH W 171 | 46.578 | 59.161 | | 1.00 77.64 1.00 51.18 | W W | 0 |
| | ATOM | | 0 | HOH W 172 | 48.228 | 52.442 | 14.549 -7.042 | 1.00 51.18 1.00 87.49 | W | 0 |
| | MOTA | 6417 | 0 | HOH W 173 | 70.197 | 2.753 | -7.042 -6.765 | 1.00 67.49 | W | ŏ |
| | ATOM | | 0 | HOH W 174 | 64.004 | 2.450 -4.990 | -18.564 | 1.00 72.72 | W | ŏ |
| 5 | MOTA | | 0 | HOH W 175 | 42.696 18.059 | | -13.442 | 1.00101.30 | W | Ö |
| | MOTA | | 0 | HOH W 177 | 15.355 | | -29.333 | 1.00 68.26 | W | O |
| | ATOM | | 0 | HOH W 180 HOH W 181 | 35.274 | | -15.496 | 1.00 81.17 | W | 0 |
| | ATOM | | 0 | HOH W 181 HOH W 182 | 37.734 | | -17.674 | 1.00 76.65 | W | 0 |
| | ATOM | | 0 | HOH W 183 | 4.398 | | -27.101 | 1.00 73.23 | W | 0 |
| 10 | ATOM | | 0 | HOH W 183 | 25.726 | 62.296 | 18.755 | 1.00 68.08 | M | 0 |
| | ATOM | 6425 | 0 | HOH W 185 | 55.967 | 5.969 | 6.509 | 1.00 63.28 | W | 0 |
| | MOTA | 6426 6427 | 0 | HOH W 186 | 52.635 | 32.458 | 16.778 | 1.00 64.30 | W | 0 |
| | MOTA | 6428 | 0 | HOH W 187 | 42.187 | 61.267 | 1.486 | 1.00 63.63 | M | 0 |
| 45 | ATOM ATOM | 6429 | Ö | HOH W 188 | 54.080 | 67.804 | 9.345 | 1.00 73.07 | W | 0 |
| 15 | ATOM | 6430 | ŏ | HOH W 191 | 39.373 | 49.817 | 15.778 | 1.00 73.96 | M | 0 |
| | ATOM | 6431 | ŏ | HOH W 192 | 30.145 | 48.697 | 18.491 | 1.00 67.43 | W | 0 |
| | ATOM | 6432 | ŏ | HOH W 193 | 58.517 | | -10.692 | 1.00 64.51 | M | 0 |
| | ATOM | 6433 | ŏ | HOH W 194 | 66.066 | 47.014 | 5.586 | 1.00 70.05 | W | 0 |
| 20 | ATOM | 6434 | ō | HOH W 195 | 60.708 | 45.623 | -2.248 | 1.00 54.73 | W | 0 |
| 20 | ATOM | 6435 | 0 | HOH W 197 | 40.532 | 56.318 | -5.957 | 1.00 61.38 | W | 0 |
| | ATOM | 6436 | 0 | HOH W 198 | 59.085 | 42.157 | -5.617 | 1.00 63.62 | M | 0 |
| | ATOM | 6437 | 0 | HOH W 199 | 58.018 | 28.117 | 9.569 | 1.00 59.02 1.00 91.05 | W | ŏ |
| | MOTA | 6438 | 0 | HOH W 200 | 62.084 | 19.823 | -10.491 | 1.00 91.05 | W | ő |
| 25 | ATOM | 6439 | 0 | HOH W 201 | 71.317 | -2.871 | 5.295 -4.399 | 1.00 67.04 | W | ŏ |
| | ATOM | 6440 | 0 | HOH W 202 | 25.844 | 56.209 | 13.305 | 1.00 78.61 | W | ŏ |
| | MOTA | 6441 | 0 | HOH W 203 | 50.532 | 31.124 43.277 | 5.774 | 1.00 53.65 | W | ŏ |
| | MOTA | 6442 | 0 | HOH W 204 | 25.247 | 36.272 | -4.050 | 1.00 82.87 | W | O |
| | MOTA | 6443 | 0 | HOH W 205 | 53.767 53.294 | 78.768 | | 1.00 56.03 | W | 0 |
| 30 | MOTA | 6444 | 0 | HOH W 206 | 47.425 | 27.397 | 11.529 | 1.00 75.72 | W | 0 |
| | MOTA | 6445 | 0 | нон W 207 нон W 208 | 51.605 | 34.818 | | 1.00 75.55 | W | 0 |
| | MOTA | 6446 | 0 | HOH W 208 | 43.903 | 15.886 | | 1.00 74.13 | W | 0 |
| | MOTA | 6447 | 0 | HOH W 210 | 46.556 | 14.040 | | 1.00 91.12 | W | 0 |
| | MOTA | 6448 | 0 | HOH W 210 | 40.263 | 22.624 | | 1.00 89.07 | W | 0 |
| 35 | MOTA | 6449 | 0 | HOH W 211 | 55.658 | 6.616 | | 1.00 84.65 | W | 0 |
| | MOTA | 6450 6451 | 0 | HOH W 214 | 58.186 | 32.450 | | 1.00 61.74 | M | 0 |
| | MOTA | 6452 | Ö | HOH W 215 | 58.141 | 37.758 | | 1.00 61.98 | W | 0 |
| | MOTA MOTA | 6453 | ŏ | HOH W 216 | 56.966 | 35.250 | 2.674 | 1.00 57.55 | W | 0 |
| 40 | ATOM | 6454 | ŏ | HOH W 217 | 55.211 | 32.727 | | 1.00 53.03 | M | 0 |
| 40 | ATOM | 6455 | ŏ | HOH W 218 | 52.367 | 31.257 | -12.864 | 1.00 74.72 | M | 0 |
| | ATOM | 6456 | ō | HOH W 220 | 56.462 | 36.886 | | 1.00 63.55 | W | 0 |
| | ATOM | 6457 | Ō | HOH W 224 | 29.998 | 24.261 | | 1.00 60.64 | M | 0 |
| | ATOM | 6458 | 0 | HOH W 225 | 24.007 | 3.807 | | 1.00 62.70 | W | 0 |
| 45 | ATOM | 6459 | 0 | HOH W 226 | 45.167 | 21.855 | | 1.00 88.68 1.00 56.13 | M | ő |
| | ATOM | 6460 | 0 | HOH W 227 | 53.676 | 66.697 | | | W | Õ |
| | ATOM | 6461 | 0 | HOH W 229 | 51.011 | 64.329 | | 1.00 95.18 1.00 80.36 | W | ŏ |
| | MOTA | 6462 | 0 | HOH W 230 | 39.248 | 30.285 | | - · | W | ŏ |
| | MOTA | 6463 | 0 | HOH W 231 | 44.473 | 38.407 | 7 17.076 | | W | ŏ |
| 50 | MOTA | 6464 | 0 | HOH W 235 | 25.679 | 2.134 | 1 -15.868) -21.135 | | W | ŏ |
| | MOTA | 6465 | 0 | HOH W 236 | 32.236 | 28.315 | 6.252 | | W | Ō |
| | MOTA | 6466 | 0 | HOH W 237 | 34.413 | | | | W | 0 |
| | MOTA | 6467 | 0 | HOH W 238 | 27.724 | | | | W | O |
| | MOTA | 6468 | 0 | HOH W 239 | 56.205 | | | | W | 0 |
| 55 | MOTA | 6469 | 0 | HOH W 240 | 66.188 63.285 | | | | W | 0 |
| | MOTA | 6470 | 0 | HOH W 242 | 60.113 | | | | W | 0 |
| | MOTA | 6471 | 0 | HOH W 243 | 57.113 | | | | M | 0 |
| | MOTA | 6472 | 0 | HOH W 244 | 46.457 | | | | M | 0 |
| | MOTA | 6473 | 0 | HOH W 245 | 42.305 | | | | W | 0 |
| 60 | MOTA | 6474 | 0 | HOH W 246 | 32.141 | | | | W | 0 |
| | ATOM | 6475 | 0 | нон W 247 нон W 248 | 58.909 | | | | M | 0 |
| | MOTA | 6476 | 0 | HOH W 240 | 38.763 | | | | M | 0 |
| | MOTA | 6477 | 0 | нон W 249 нон W 250 | 39.214 | 62.95 | | 1.00 75.29 | M | 0 |
| | MOTA | 6478 | 0 | HOH W 250 | 60.671 | | | 1.00 55.23 | W | 0 |
| 65 | MOTA | 6479 | 0 | HOH W 252 | 38.380 | | | 1.00 74.82 | W | 0 |
| | MOTA | 6480 | | HOH W 254 | 44.133 | | | 3 1.00 87.18 | W | 0 |
| | MOTA | 6481 6482 | | HOH W 255 | 32.114 | | | 2 1.00 84.19 | W | 0 |
| | MOTA ATOM | 6483 | | HOH W 256 | 46.385 | 47.10 | 1 -10.075 | 5 1.00 80.35 | W | 0 |
| | ATOM | 0-±00 | | 200 | 070 | | | | | |

^aAmino acids residues of the light (L) and heavy (H) chains are numbered according to the Chothia numbering system as shown in Tables 6 and 7, respectively (Al-Lazikani *et al.*, *Jour. Mol. Biol.* 273;927-948, 1997). Amino acid residues of IL-13 (I) are numbered as shown in SEQ ID NO:4 (FIG. 2B). Amino acid residues of IL-13Rα1 are numbered as shown in SEQ ID NO:12 (FIG. 14).

Other embodiments are in the claims

^bColumns are labeled according to Protein Data Bank Format, Version 2.2

WHAT IS CLAIMED IS:

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1. A crystalline antibody, wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

- 2. The crystalline antibody of claim 1, wherein the crystalline antibody has space group $P2_12_12_1$.
 - 3. The crystalline antibody according to any one of claims 1 or 2, wherein the crystalline antibody has unit cell dimensions a=54.4, b=98.0, c=108.5, and $\alpha=\beta=\gamma=90^{\circ}$.
 - 4. The crystalline antibody according to any one of claims 1-3, wherein the antibody is from a mammal.
 - 5. The crystalline antibody according to any one of claims 1-4, wherein the antibody is from a mouse, rat, rabbit, or goat.
 - 6. The crystalline antibody according to any one of claims 1-5, further comprising an IL-13 polypeptide bound to the antibody.
 - 7. The crystalline antibody of claim 6, further comprising an IL-13R α 1 polypeptide bound to the IL-13 polypeptide.
 - 8. The crystalline antibody according to any one of claims 1-7, wherein the antibody comprises a polypeptide including the amino acid sequence of SEQ ID NO:1.
 - 9. The crystalline antibody according to any one of claims 1-8, wherein the antibody comprises a polypeptide including the amino acid sequence of SEQ ID NO:2.

10. The crystalline antibody according to any one of claims 1-9, wherein the antibody is a monoclonal antibody.

- 11. The crystalline antibody according to any one of claims 1-10, wherein the antibody is mAb13.2.
 - 12. The crystalline antibody according to any one of claims 1-11, wherein the antibody is an mAb13.2 Fab fragment.
- 13. The crystalline antibody according to any one of claims 1-12, wherein the antibody is capable of binding to a region of IL-13 that binds to an IL-4R polypeptide *in vivo*.
 - 14. The crystalline antibody according to any one of claims 1-13, wherein the crystalline antibody can diffract X-rays to a resolution of at least about 3.5 Å.
 - 15. The crystalline antibody according to any one of claims 1-14, wherein the crystalline antibody comprises the structural coordinates of Table 10, +/- a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.
 - 16. The crystalline antibody according to any one of claims 1-15, wherein: the light chain of the antibody comprises the amino acid sequence of SEQ ID NO:1;
 - the heavy chain of the antibody comprises the amino acid sequence of SEQ ID $\,$ NO:2; and

the crystalline antibody diffracts X-rays to a resolution of at least about 3.5 Å.

17. A crystalline composition that comprises an antibody, wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

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18. The crystalline composition of claim 17, further comprising at least one water molecule.

- 19. The crystalline composition according to any one of claims 17 or 18, further comprising a salt or zinc.
 - 20. The crystalline composition according to any one of claims 17-19, further comprising an IL-13 polypeptide bound to the anti-IL-13 antibody or Fab fragment.
- 21. The crystalline composition of claim 20, further comprising an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.
 - 22. A crystalline complex, comprising:

an IL-13 polypeptide; and

an antibody,

wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

- 23. The crystalline complex of claim 22, wherein the crystalline complex has space group P2₁3.
 - 24. The crystalline complex according to any one of claims 22 or 23, wherein the crystalline complex has unit cell dimensions a = b = c = 125.3 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

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- 25. The crystalline complex according to any one of claims 22-24, wherein the antibody is from a mammal.
- 26. The crystalline complex according to any one of claims 22-25, wherein the antibody is from a mouse.

27. The crystalline complex according to any one of claims 22-26, wherein the IL-13 polypeptide is from a mammal.

28. The crystalline complex according to any one of claims 22-27, wherein the IL-13 polypeptide is from a human.

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- 29. The crystalline complex according to any one of claims 22-28, wherein the antibody comprises a polypeptide including the amino acid sequence of SEQ ID NO:1.
- 30. The crystalline complex according to any one of claims 22-29, wherein the antibody comprises a polypeptide including the amino acid sequence of SEQ ID NO:2.
 - 31. The crystalline complex according to any one of claims 22-30, wherein the antibody is a monoclonal antibody.
 - 32. The crystalline complex according to any one of claims 22-31, wherein the antibody is mAb13.2.
- 33. The crystalline complex according to any one of claims 22-32, wherein the antibody is an mAb13.2 Fab fragment.
 - 34. The crystalline complex according to any one of claims 22-33, wherein the antibody is bound to a region of the IL-13 polypeptide that binds to an IL-4R polypeptide in vivo.
 - 35. The crystalline complex according to any one of claims 22-34, wherein the IL-13 polypeptide comprises a region that binds to an IL-4R polypeptide.
- 36. The crystalline complex according to any one of claims 22-35, wherein the IL-13 polypeptide comprises the amino acid sequence of SEQ ID NO:4.

37. The crystalline complex according to any one of claims 22-36, wherein the antibody interacts with one or more of residues Ser7, Thr8, Ala9, Glu12, Leu48, Glu49, Ile52, Asn53, Arg65, Ser68, Gly69, Phe70, Cys71, Pro72, His73, Lys74, and Arg86 as defined by the amino acid sequence of SEQ ID NO:4.

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- 38. The crystalline complex according to any one of claims 22-37, wherein the IL-13 polypeptide interacts with one or more of residues Asn31, Tyr32, Lys34, Arg54, Asn96, Asp98, and Trp100 as defined by the amino acid sequence of SEQ ID NO:1 and Ile30, Ser31, Ala33, Trp47, Ser50, Ser52, Ser53, Tyr58, Leu98, Asp99, Gly100, Tyr101, Tyr102, and Phe103 as defined by the amino acid sequence of SEQ ID NO:2.
- 39. The crystalline complex according to any one of claims 22-38, wherein the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.
- 40. The crystalline complex according to any one of claims 22-39, wherein the crystalline complex comprises the structural coordinates of Table 11, +/- a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.
- 41. The crystalline complex according to any one of claims 22-40, further comprising an IL-13Rα1 polypeptide.
 - 42. A crystalline complex, comprising:

an IL-13Ra1 polypeptide; and

an IL-13 polypeptide.

- 43. The crystalline complex of claim 42, wherein the crystalline complex has space group I4.
- 44. The crystalline complex according to any one of claims 42 or 43, wherein the crystalline complex has unit cell dimensions a = b = 164.9 Å, c = 74.8 Å and $\alpha = \beta = \gamma = 90^{\circ}$.

45. The crystalline complex according to any one of claims 42, 43, or 44, further comprising an antibody,

wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

- 46. The crystalline complex of claim 45, wherein the antibody is from a mammal.
- 47. The crystalline complex according to any one of claims 45 or 46, wherein the antibody is from a mouse.
 - 48. The crystalline complex according to any one of claims 42-47, wherein the IL-13 polypeptide is from a mammal.
 - 49. The crystalline complex according to any one of claims 42-48, wherein the IL-13 polypeptide is from a human.
 - 50. The crystalline complex according to any one of claims 45 or 46, wherein the antibody is a monoclonal antibody.
 - 51. The crystalline complex according to any one of claims 45 or 46, wherein the antibody is mAb13.2.
 - 52. The crystalline complex according to any one of claims 45 or 46, wherein the antibody is an mAb13.2 Fab fragment.
 - 53. The crystalline complex according to any one of claims 45 or 46, wherein the antibody is bound to a region of the IL-13 polypeptide that binds to an IL-4R polypeptide in vivo.

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54. The crystalline complex according to any one of claims 42-53, wherein the IL-13 polypeptide comprises a region that binds to an IL-4R polypeptide.

- 55. The crystalline complex according to any one of claims 42-54, wherein the
 IL-13Rα1 polypeptide is from a mammal.
 - 56. The crystalline complex according to any one of claims 42-55, wherein the IL-13Rα1 polypeptide is from a human
- 57. The crystalline complex according to any one of claims 42-56, wherein the IL-13 polypeptide comprises the amino acid sequence of SEQ ID NO:4.

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- 58. The crystalline complex according to any one of claims 42-57, wherein the IL-13Rα1 polypeptide comprises the amino acid sequence of SEQ ID NO:12.
- 59. The crystalline complex according to any one of claims 44 or 46, wherein the antibody interacts with one or more of residues Ser7, Thr8, Ala9, Glu12, Leu48, Glu49, Ile52, Asn53, Arg65, Ser68, Gly69, Phe70, Cys71, Pro72, His73, Lys74, and Arg86 as defined by the amino acid sequence of SEQ ID NO:4.
- 60. The crystalline complex according to any one of claims 45 or 46, wherein the IL-13 polypeptide interacts with one or more of residues Asn31, Tyr32, Lys34, Arg54, Asn96, Asp98, and Trp100 as defined by the amino acid sequence of SEQ ID NO:1 and Ile30, Ser31, Ala33, Trp47, Ser50, Ser52, Ser53, Tyr58, Leu98, Asp99, Gly100, Tyr101, Tyr102, and Phe103 as defined by the amino acid sequence of SEQ ID NO:2.
- 61. The crystalline complex according to any one of claims 42-60, wherein the IL-13 polypeptide interacts with one or more of residues Ile254, Ser255, Arg256, Lys318, Cys320, Tyr321, Lys76, Lys77, Ile78, and Ala79 as defined by the amino acid sequence of SEQ ID NO:12.

62. The crystalline complex according to any one of claims 42-59, wherein the IL-13Rα1 polypeptide interacts with one or more of residues Arg11, Glu12, Leu13, Ile14, Glu15, Thr88, Lys89, Ile90, Glu91, Lys104, Lys105, Leu106, Phe107, and Arg108, as defined by the amino acid sequence of SEQ ID NO:4.

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- 63. The crystalline complex according to any one of claims 42-62, wherein the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.
- 64. The crystalline complex according to any one of claims 42-63, wherein the crystalline complex comprises the structural coordinates of Table 12, +/- a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.
 - 65. A method comprising:

using a three-dimensional model of an antibody to design an agent that interacts with an IL-13 polypeptide,

wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

- 66. The method of claim 65, wherein the three-dimensional model comprises a CDR of the antibody.
 - 67. The method according to any one of claims 65 or 66, wherein the antibody is a Fab fragment of an anti-IL-13 antibody.
 - 68. The method according to any one of claims 65-67, wherein the antibody comprises a light chain polypeptide including the amino acid sequence of SEQ ID NO:1, and a heavy chain polypeptide including the amino acid sequence of SEQ ID NO:2.
 - 69. The method according to any one of claims 65-68, wherein the antibody is mAb13.2.

70. The method according to any one of claims 65-69, wherein the antibody is an mAb13.2 Fab fragment.

- 71. The method according to any one of claims 65-70, wherein the three-dimensional model comprises structural coordinates of atoms of the antibody.
 - 72. The method of claim 71, wherein the structural coordinates are experimentally determined coordinates.
- 73. The method according to any one of claims 65-72, wherein the three-dimensional model comprises structural coordinates of an atom selected from the group consisting of atoms of amino acids Asn31, Tyr32, Lys34, Arg54, Asn96, Asp98, and Trp100 as defined by the amino acid sequence of SEQ ID NO:1, and Ile30, Ser31, Ala33, Trp47, Ser50, Ser52, Ser53, Tyr58, Leu98, Asp99, Gly100, Tyr101, Tyr102, and Phe103 as defined by the amino acid sequence of SEQ ID NO:2.
- 74. The method according to any one of claims 65-73, wherein the agent binds a region of the IL-13 polypeptide that binds an IL-4R polypeptide *in vivo*.
- 75. The method of claim 74, wherein the IL-4R polypeptide is an IL-4R α polypeptide.
 - 76. The method according to any one of claims 65-75, wherein the three-dimensional model comprises an IL-13 polypeptide bound to the antibody.
 - 77. The method of claim 76, wherein the three-dimensional model further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.
 - 78. A method comprising:

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using a three-dimensional model of an IL-13 polypeptide to design an agent that interacts with the IL-13 polypeptide.

79. The method of claim 78, wherein the three-dimensional model further comprises an antibody bound to the IL-13 polypeptide, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

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80. The method of claim 79, wherein the three-dimensional model comprises structural coordinates of atoms of the antibody.

81. The method according to any one of claims 78-807, wherein the three-dimensional model comprises a region of the IL-13 polypeptide that binds to an IL-4R polypeptide *in vivo*.

82. The method according to any one of claims 78-81, wherein the agent inhibits binding of the IL-13 polypeptide to an IL-4R polypeptide.

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83. The method according to any one of claims 75-79, wherein the three-dimensional model comprises structural coordinates of atoms of the IL-13 polypeptide.

84. The method of claim 83, wherein the structural coordinates are experimentally determined coordinates.

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85. The method according to any one of claims 83 or 84, wherein the structural coordinates are according to Table 11 +/- a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

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86. The method according to any one of claims 78-85, wherein the three-dimensional model comprises structural coordinates of an atom selected from the group consisting of atoms of amino acids Glu49, Asn53, Ser68, Gly69, Phe70, Cys71, Pro72, His73, Lys74, and Arg86 of the IL-13 polypeptide as defined by the amino acid sequence of SEQ ID NO:4.

87. The method according to any one of claims 78-86, wherein the three-dimensional model further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.

- 88. The method of claim 87, wherein the three-dimensional model comprises structural coordinates of atoms of the IL-13Rα1 polypeptide.
 - 89. A method comprising:

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using a three-dimensional model of an IL-13 polypeptide bound to an IL-13Rα1 polypeptide to design an agent that interacts with the IL-13 polypeptide.

- 90. The method of claim 89, wherein the three-dimensional model further comprises an antibody bound to the IL-13 polypeptide, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.
- 91. The method according to any one of claims 89 or 90, wherein the agent inhibits binding of the IL-13 polypeptide to an IL-4R polypeptide.
- 92. The method according to any one of claims 89-91, wherein the three-dimensional model comprises structural coordinates of atoms of the IL-13 polypeptide and the IL-13Ral polypeptide.
- 93. The method of claim 92, wherein the structural coordinates are experimentally determined coordinates.
- 94. The method according to any one of claims 92 or 93, wherein the structural coordinates are according to Table 12 +/- a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.
 - 95. A method, comprising:

selecting an agent by performing rational drug design with a three-dimensional structure of a crystalline complex that comprises an IL-13 polypeptide;

contacting the agent with an IL-13 polypeptide; and detecting the ability of the agent to bind the IL-13 polypeptide.

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96. The method of claim 95, wherein the crystalline complex of the three-dimensional structure further comprises an antibody bound to the IL-13 polypeptide, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

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97. The method of claim 96, wherein the anti-IL-13 antibody or Fab fragment of an anti-IL-13 antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

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98. The method according to any one of claims 95-97, wherein the agent is selected via computer modeling.

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99. The method according to any one of claims 95-98, wherein the three-dimensional structure comprises structural coordinates of Table 11, \pm a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

100. The method according to any one of claims 95-99, wherein the crystalline complex of the three-dimensional structure further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.

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101. The method according to any one of claims 95-100, wherein the three-dimensional structure comprises structural coordinates of Table 12, \pm a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

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102. The method according to any one of claims 95-101, further comprising obtaining the agent.

103. The method according to any one of claims 95-102, further comprising: obtaining a supplemental crystalline complex comprising the IL-13 polypeptide and the agent;

determining the three-dimensional structure of the supplemental crystalline complex;

selecting a second agent by performing rational drug design with the threedimensional structure of the supplemental crystalline complex;

contacting the second agent with the IL-13 polypeptide; and detecting the ability of the second agent to bind the IL-13 polypeptide.

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- 104. The method of claim 103, wherein the second agent is selected via computer modeling.
- 105. The method according to any one of claims 103 or 104, further comprising detecting an ability of the second agent to inhibit IL-13 activity.
 - 106. A method, comprising:

contacting an IL-13 polypeptide with an antibody to form a composition; and crystallizing the composition to form a crystalline complex in which the antibody is bound to the IL-13 polypeptide,

wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

- 107. The method of claim 106, wherein the method includes using vapor diffusion.
- 108. The method according to any one of claims 106 or 107, wherein the antibody is mAb13.2.

109. The method according to any one of claims 106-108, wherein the antibody is a mAb13.2 Fab fragment.

110. A method, comprising:

contacting an IL-13 polypeptide with an antibody and an IL-13R α 1 polypeptide to form a composition; and

crystallizing the composition to form a crystalline complex in which the antibody and the IL-13Ra1 polypeptide are each bound to the IL-13 polypeptide,

wherein the antibody comprises an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

- 111. The method of claim 110, wherein the method includes using vapor diffusion.
- 112. The method according to any one of claims 110-111, wherein the antibody is mAb13.2.
- 113. The method according to any one of claims 110-112, wherein the antibody is an mAb13.2 Fab fragment.
- 114. A software system, comprising instructions for causing a computer system to:

accept information relating to a structure of an IL-13 polypeptide bound to an antibody, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody;

accept information relating to a candidate agent; and determine binding characteristics of the candidate agent to the IL-13 polypeptide, wherein the determination is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent.

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115. The software system of claim 114, wherein the structure of the IL-13 polypeptide bound to the antibody is a crystal structure.

116. The software system of claim 115, wherein the crystal structure comprises the structural coordinates of Table 11, \pm a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.

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- 117. The software system according to any one of claims 106-108, wherein the structure of the IL-13 polypeptide bound to the antibody further comprises an IL-13R α 1 polypeptide bound to the IL-13 polypeptide.
- 118. The software system of claim 117, wherein the structure of the IL-13 polypeptide bound to the antibody and the IL-13Ra1 polypeptide bound to the IL-13 polypeptide is a crystal structure.
- 119. The software system of claim 118, wherein the crystal structure comprises the structural coordinates of Table 12, \pm a root mean square deviation for alpha carbon atoms of not more than 1.5 Å.
- 120. The software system according to any one of claims 114-119, further comprising instructions for causing the computer system to:

apply information from a database, the information relating to candidate agents; and

identify a candidate agent in the database that can bind the IL-13 polypeptide, wherein the identification is based on the information relating to the structure of the IL-13 polypeptide and information relating to the candidate agent.

121. The software system according to any one of claims 114-120, further comprising instructions for causing the computer system to model the binding characteristics of the candidate agent with the IL-13 polypeptide.

122. A computer program residing on a computer readable medium having a plurality of instructions stored thereon, which, when executed by one or more processors, cause the one or more processors to:

accept information relating to a structure of an IL-13 polypeptide bound to an antibody, the antibody comprising an anti-IL-13 polypeptide or a Fab fragment of an anti-IL-13 antibody;

accept information relating to a candidate agent; and determine binding characteristics of the candidate agent to the IL-13 polypeptide, wherein the determination is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent.

123. The computer program of claim 122, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.

124. A method, comprising:

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accepting information relating to the structure of an IL-13 polypeptide bound to an antibody, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody; and

modeling the binding characteristics of the IL-13 polypeptide with a candidate agent,

wherein the method is implemented by a software system.

- 125. The method of claim 124, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.
- 126. The method according to any one of claims 124 or 125, further comprising applying information from a database of candidate agents to identify a candidate agent that can bind the IL-13 polypeptide,

wherein the identification is based on the information relating to the structure of the IL-13 polypeptide and information relating to the candidate agent.

127. A computer program residing on a computer readable medium having a plurality of instructions stored thereon, which, when executed by one or more processors, cause the one or more processors to:

accept information relating to the structure of an IL-13 polypeptide bound to an antibody, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody; and

model the binding characteristics of the IL-13 polypeptide with a candidate agent.

128. The computer program of claim 127, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.

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129. The computer program according to any one of claims 127 or 128, further comprising instructions which cause the one or more processors to:

apply information from a database, the information relating to candidate agents; and

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identify a candidate agent in the database that can bind the IL-13 polypeptide, wherein the identification is based on the information relating to the structure of the IL-13 polypeptide.

- 130. The computer program according to any one of claims 127-129, further comprising instructions which cause the one or more processors to model the binding characteristics of the candidate agent with the IL-13 polypeptide.
- 131. A software system, comprising instructions for causing a computer system to:

accept information relating to the structure of an IL-13 polypeptide bound to an antibody, the antibody comprising an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody; and

model the binding characteristics of the IL-13 polypeptide with a candidate agent.

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- 132. The method of claim 131, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13R α 1 polypeptide bound to the IL-13 polypeptide.
- 133. A crystalline antibody, wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.
 - 134. A crystalline composition that comprises an antibody, wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds in vivo.
 - 135. A crystalline complex, comprising:

an IL-13 polypeptide; and

an antibody,

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wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

136. A crystalline complex, comprising:

an IL-13 polypeptide;

an IL-13Ra1 polypeptide; and

an antibody,

wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

137. A method, comprising:

using a three-dimensional model of an antibody to design an agent that interacts with an IL-13 polypeptide,

wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.

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138. The method of claim 137, wherein the three-dimensional model comprises structural coordinates of atoms of the antibody.

139. A method, comprising:

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contacting an IL-13 polypeptide with an antibody to form a composition; and crystallizing the composition to form a crystalline complex in which the antibody is bound to the IL-13 polypeptide,

wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

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140. A method, comprising:

contacting an IL-13 polypeptide with an antibody and an IL-13R α 1 polypeptide to form a composition; and

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crystallizing the composition to form a crystalline complex in which the antibody and the IL-13Ra1 polypeptide are each bound to the IL-13 polypeptide,

wherein the antibody is capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*, and the crystalline complex can diffract X-rays to a resolution of at least about 3.5 Å.

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141. A software system, comprising instructions for causing a computer system to:

accept information relating to a structure of an IL-13 polypeptide bound to an antibody, the antibody being capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*;

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accept information relating to a candidate agent; and

determine binding characteristics of the candidate agent to the IL-13 polypeptide, wherein the determination is based on the information relating to the structure of the IL-13 polypeptide and the information relating to the candidate agent.

5 142. The software system of claim 141, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.

143. A computer program residing on a computer readable medium having a plurality of instructions stored thereon, which, when executed by one or more processors, cause the one or more processors to:

accept information relating to a structure of an IL-13 polypeptide bound to an antibody, the antibody being capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*;

accept information relating to a candidate agent; and
determine binding characteristics of the candidate agent to the IL-13 polypeptide,
wherein the determination is based on the information relating to the structure of
the IL-13 polypeptide and the information relating to the candidate agent.

144. The computer program of claim 143, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13R α 1 polypeptide bound to the IL-13 polypeptide.

145. A method, comprising:

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accepting information relating to the structure of an IL-13 polypeptide bound to a an antibody, the antibody being capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*; and

modeling the binding characteristics of the IL-13 polypeptide with a candidate agent,

wherein the method is implemented by a software system.

146. The method of claim 145, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13R α 1 polypeptide bound to the IL-13 polypeptide.

147. A computer program residing on a computer readable medium having a plurality of instructions stored thereon, which, when executed by one or more processors, cause the one or more processors to:

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accept information relating to the structure of an IL-13 polypeptide bound to an antibody, the antibody being capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*; and

model the binding characteristics of the IL-13 polypeptide with a candidate agent.

- 148. The computer program of claim 147, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13Rα1 polypeptide bound to the IL-13 polypeptide.
- 149. A software system, comprising instructions for causing a computer system to:

accept information relating to the structure of an IL-13 polypeptide bound to an antibody, the antibody being capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*; and

model the binding characteristics of the IL-13 polypeptide with a candidate agent.

- 150. The software system of claim 149, wherein the structure of the IL-13 polypeptide bound to an antibody further comprises an IL-13R α 1 polypeptide bound to the IL-13 polypeptide.
- 151. A method of modulating IL-13 activity in a subject, comprising: using rational drug design to select an agent that is capable of modulating IL-13 activity; and

administering a therapeutically effective amount of the agent to the subject.

152. The method of claim 151, wherein the rational drug design includes using a three-dimensional structure of a crystalline complex that comprises an IL-13 polypeptide.

153. The method of claim 152, wherein the crystalline complex further comprises an antibody, the antibody being an anti-IL-13 antibody or a Fab fragment of an anti-IL-13 antibody.

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- 154. The method according to any one of claims 152 or 153, wherein the crystalline complex further comprises an antibody, the antibody being capable of binding a site of an IL-13 polypeptide to which an IL-4R polypeptide binds *in vivo*.
 - 155. The method according to any one of claims 152-154, wherein the crystalline complex further comprises an IL-13R α 1 polypeptide.

156. A method of treating a subject having a condition associated with IL-13 activity, comprising:

using rational drug design to select an agent that is capable of effecting IL-13 activity; and

administering a therapeutically effective amount of the agent to a subject in need thereof.

- 157. The method of claim 156, wherein the condition is asthma.
- 158. The method according to any one of claims 156 or 157, wherein the condition is allergic asthma or nonallergic asthma.
- 159. The method of claim 156, wherein the condition comprises at least one condition selected from the group consisting of cancer, airway inflammation, eosinophilia, fibrosis, excess mucus production, an inflammatory condition of the skin,

gastrointestinal organs, blood vessels or connective tissue, and an autoimmune condition of the skin, gastrointestinal organs, blood vessels, or connective tissue.

160. The method of claim 156, wherein the condition comprises at least one condition selected from the group consisting of chronic obstructive pulmonary disorder, cystic fibrosis, pulmonary fibrosis, allergic rhinitis, atopic dermatitis, inflammatory bowel disease, Crohn's disease, cirrhosis, scleroderma, or Hodgkin's lymphoma.

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161. A method of prophylactically treating a subject susceptible to a condition associated with IL-13 activity, comprising:

determining that the subject is susceptible to the condition associated with IL-13 activity;

using rational drug design to select an agent that is capable of effecting IL-13 activity; and

administering a therapeutically effective amount of the agent to the subject.

- 162. The method of claim 161, wherein the condition is asthma.
- 163. The method according to any one of claims 161 or 162, wherein the condition is allergic asthma or nonallergic asthma.
- 164. The method of claim 161, wherein the condition comprises at least one condition selected from the group consisting of cancer, airway inflammation, eosinophilia, fibrosis, excess mucus production, an inflammatory condition of the skin, gastrointestinal organs, blood vessels or connective tissue, and an autoimmune condition of the skin, gastrointestinal organs, blood vessels, or connective tissue.
- 165. The method of claim 161, wherein the condition comprises at least one condition selected from the group consisting of chronic obstructive pulmonary disorder, cystic fibrosis, pulmonary fibrosis, allergic rhinitis, atopic dermatitis, inflammatory bowel disease, Crohn's disease, cirrhosis, scleroderma, or Hodgkin's lymphoma.

166. The method according to any one of claims 161-165, wherein the agent binds to the IL-13 polypeptide by interacting to within about 2.0Å with one or more of amino acids Glu49, Asn53, Gly69, Pro72, His73, Lys74, and Arg86, as defined by the amino acid sequence of SEQ ID NO:4.

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- 167. Use of an agent designed or selected according to any one of claims 64-97 or 129 or 130 in the manufacture of a medicament for the prophylaxis or treatment of a condition associated with IL-13 activity.
- 168. The use according to claim 167, wherein the agent is capable of inhibiting IL-13 activity.
- 169. The use according to any one of claims 167 or 168, wherein the agent is capable of inhibiting IL-13 activity *in vivo*.
 - 170. The use according to any one of claims 167, 168, or 169, wherein the condition is asthma.
 - 171. The use according to any one of claims 167-170, wherein the condition is allergic asthma or non-allergic asthma.
 - 172. The use according to any one of claims 167-170, wherein the condition comprises at least one condition selected from the group consisting of cancer, airway inflammation, eosinophilia, fibrosis, excess mucus production, an inflammatory condition of the skin, gastrointestinal organs, blood vessels or connective tissue, and an autoimmune condition of the skin, gastrointestinal organs, blood vessels, or connective tissue.
 - 173. The use according to any one of claims 167-170, wherein the condition comprises at least one condition selected from the group consisting of chronic obstructive 297

pulmonary disorder, cystic fibrosis, pulmonary fibrosis, allergic rhinitis, atopic dermatitis, inflammatory bowel disease, Crohn's disease, cirrhosis, scleroderma, or Hodgkin's lymphoma.

- 174. The use according to any one of claims 167-173, wherein the agent binds to the IL-13 polypeptide by interacting to within about 2.0Å with one or more of amino acids Glu49, Asn53, Gly69, Pro72, His73, Lys74, and Arg86, as defined by the amino acid sequence of SEQ ID NO:4.
- 175. An agent designed or selected according to any one of claims 65-105 or 129 or 130 for use in the prophylaxis or treatment of a condition associated with IL-13 activity.
- 176. The agent of claim 175, wherein the agent is capable of inhibiting IL-13 activity.
 - 177. The agent according to any one of claims 175 or 176, wherein the agent is capable of inhibiting IL-13 activity in vivo.
 - 178. The agent according to any one of claims 175, 176, or 177, wherein the condition is asthma.

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- 179. The agent according to any one of claims 175-178, wherein the condition is allergic asthma or nonallergic asthma.
- 180. The agent according to any one of claims 175-177, wherein the condition comprises at least one condition selected from the group consisting of cancer, airway inflammation, eosinophilia, fibrosis, excess mucus production, an inflammatory condition of the skin, gastrointestinal organs, blood vessels or connective tissue, and an autoimmune condition of the skin, gastrointestinal organs, blood vessels, or connective tissue.

181. The agent according to any one of claims 175-177, wherein the condition comprises at least one condition selected from the group consisting of chronic obstructive pulmonary disorder, cystic fibrosis, pulmonary fibrosis, allergic rhinitis, atopic dermatitis, inflammatory bowel disease, Crohn's disease, cirrhosis, scleroderma, or Hodgkin's lymphoma.

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182. The agent according to any one of claims 175-181, wherein the agent binds to the IL-13 polypeptide by interacting to within about 2.0Å with one or more of amino acids Glu49, Asn53, Gly69, Pro72, His73, Lys74, and Arg86, as defined by the amino acid sequence of SEQ ID NO:4.

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| 1 | DIVITATOSPAS | LAVSLGORAT | ISCKASESVD | NYGKSLMHWY | QQKPGQSPKL |
|------------|--------------|------------|------------|------------|------------|
| = 1 | TITYRASMLES | GTPARFSGSG | SRTDFTLTIN | PVEADDVATY | YCQQSNEDPW |
| 101 | TECCCTKLET | KRADAAPTVS | IFPPSSEOLT | SGGASVVCFL | NNFYPKDINV |
| 151 | THUGGIRED | NGVINSWTDO | DSKDSTYSMS | STLTLTKDEY | ERHNSYTCEA |
| | THKTSTSPIV | | | | |

(SEQ ID NO:1) Light

FIG. 1A

| 51 101 151 | EVKLVESGGG ISSGGNTYYP YYFGFAYWGQ FPEPVTVTWN NVAHPASSTK | DSVKGRFTIS GTLVAVSAAK SGSLSSGVHT | RDNARNILYL TTPPSVYPLA | QMSSLRSEDT PGSAAQTNSM | AMYYCARLDG VTLGCLVKGY |
|------------------|--|--|--------------------------|--------------------------|--------------------------|
|------------------|--|--|--------------------------|--------------------------|--------------------------|

(SEQ ID NO:2) Heavy

FIG. 1B

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- 1 MALLLTTVIA LTCLGGFAS/P GPVP<u>PSTALR ELIEELVNIT ONO</u>KAPLCNG 51 SMVWSINLTA G<u>MYCAALESL INVSGCSAIE KTORMLSGF</u>C PHKVSAGQFS 101 SLHVRDTKIE V<u>AOFVKDLLL HLKKLFR</u>EGR FN

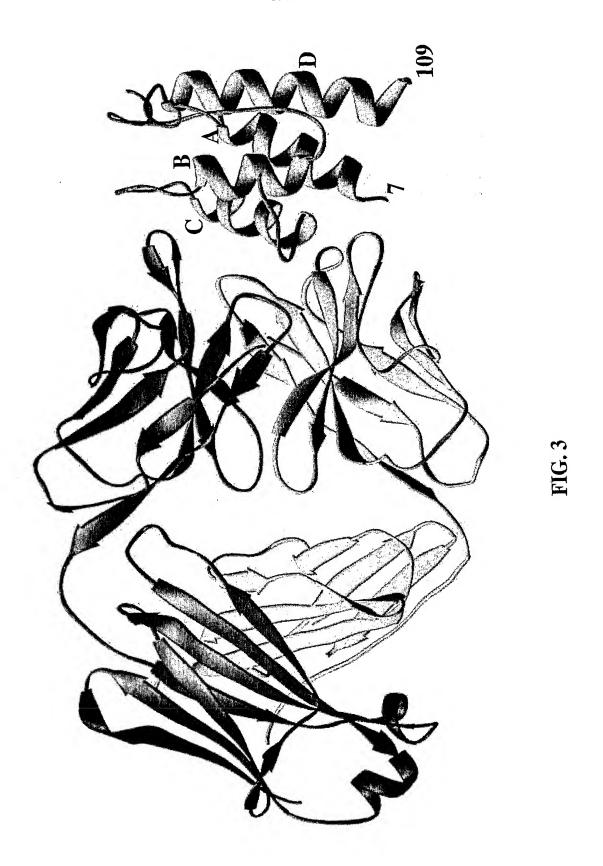
(SEQ ID NO:3) IL-13

FIG. 2A

1 PGPVP<u>PSTAL RELIEELVNI TONO</u>KAPLCN GSMVWSINLT AG<u>MYCAALES</u> 51 <u>LINVSGCSAI EKTORMLSGF</u> CPHKVSAGQF SSLHVRDTKI EV<u>AOFVKDLL</u> 101 <u>LHLKKLFR</u>EG RFN

(SEQ ID NO:4) IL-13 processed

FIG. 2B



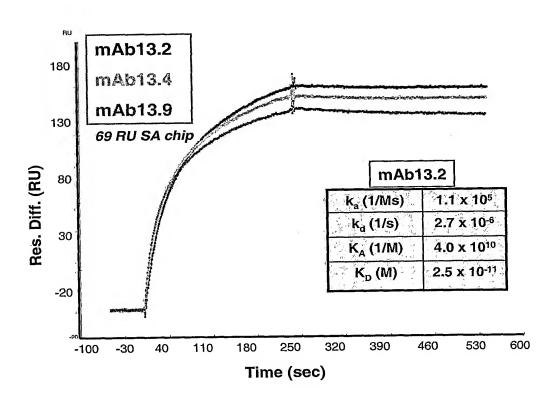


FIG. 4

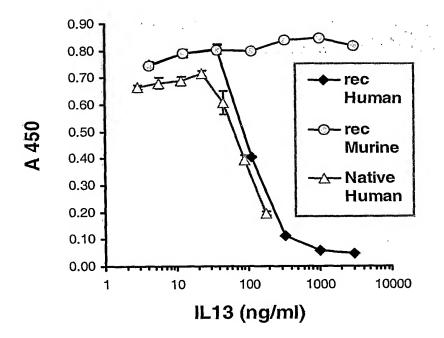


FIG. 5

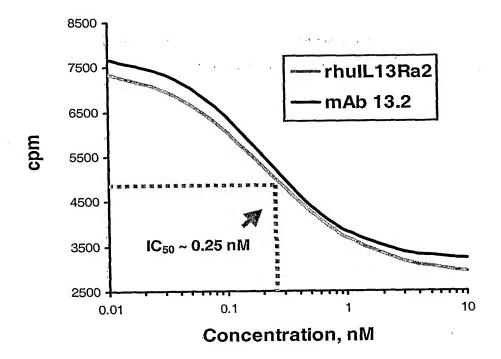
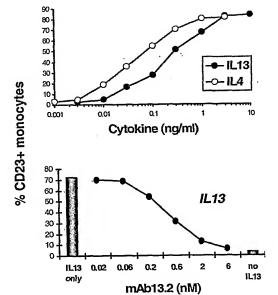


FIG. 6

FIG. 7A



Both IL13 and IL4 induce CD23 expression on human monocytes.

mAb13.2 inhibits bioactivity of IL13 but not IL4.

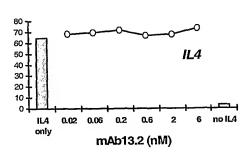


FIG. 7B

FIG. 7C

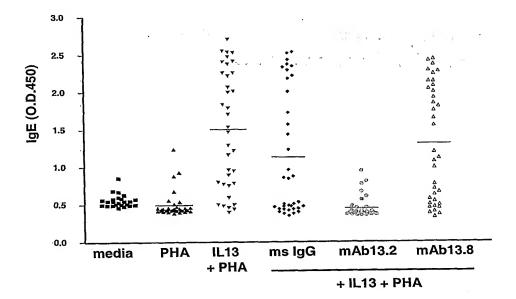
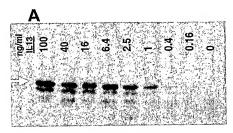


FIG. 8

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FIG. 9A



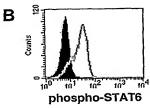
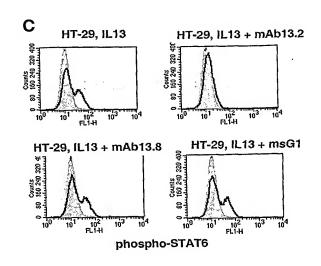


FIG. 9B

FIG. 9C





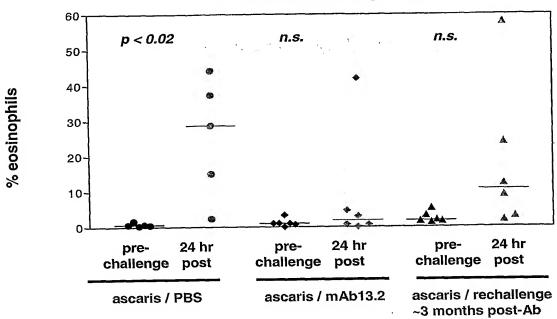
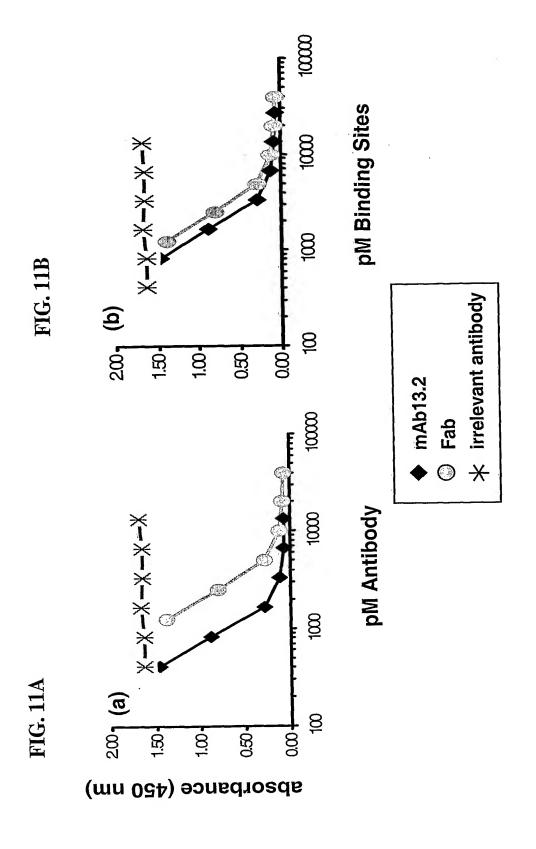
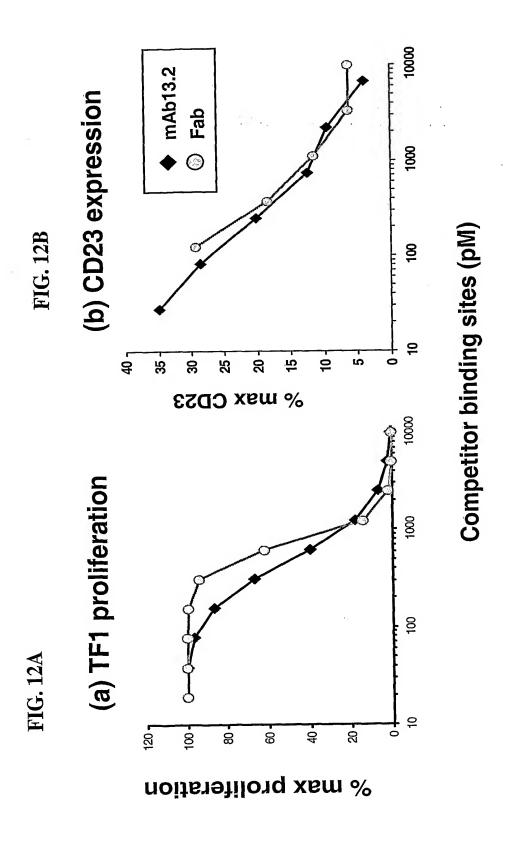


FIG. 10





| 1 | GACGAAAGGG | CCTCGTGATA | CGCCTATTTT | TATAGGTTAA | |
|------|------------|--------------|------------|--------------|------------|
| 51 | ATAATGGTTT | CTTAGACGTC | AGGTGGCACT | TTTCGGGGAA | |
| 101 | AACCCCTATT | TGTTTATTTT | TCTAAATACA | TTCAAATATG | TATCCGCTCA |
| 151 | TGAGACAATA | ACCCTGATAA | ATGCTTCAAT | AATATTGAAA | AAGGAAGAGT |
| 201 | ATGAGTATTC | AACATTTCCG | TGTCGCCCTT | ATTCCCTTTT | TTGCGGCATT |
| 251 | TTGCCTTCCT | GTTTTTGCTC | ACCCAGAAAC | GCTGGTGAAA | GTAAAAGATG |
| 301 | CTGAAGATCA | GTTGGGTGCA | CGAGTGGGTT | ACATCGAACT | GGATCTCAAC |
| 351 | AGCGGTAAGA | TCCTTGAGAG | TTTTCGCCCC | GAAGAACGTT | TTCCAATGAT |
| 401 | GAGCACTTTT | AAAGTTCTGC | TATGTGGCGC | GGTATTATCC | CGTATTGACG |
| 451 | CCGGGCAAGA | GCAACTCGGT | CGCCGCATAC | ACTATTCTCA | GAATGACTTG |
| 501 | GTTGAGTACT | CACCAGTCAC | AGAAAAGCAT | CTTACGGATG | GCATGACAGT |
| 551 | AAGAGAATTA | TGCAGTGCTG | CCATAACCAT | GAGTGATAAC | ACTGCGGCCA |
| 601 | ACTTACTTCT | GACAACGATC | GGAGGACCGA | AGGAGCTAAC | CGCTTTTTTG |
| 651 | CACAACATGG | GGGATCATGT | AACTCGCCTT | GATCGTTGGG | AACCGGAGCT |
| 701 | GAATGAAGCC | ATACCAAACG | ACGAGCGTGA | CACCACGATG | CCTGTAGCAA |
| 751 | TGGCAACAAC | GTTGCGCAAA | CTATTAACTG | GCGAACTACT | TACTCTAGCT |
| 801 | TCCCGGCAAC | AATTAATAGA | CTGGATGGAG | GCGGATAAAG | TTGCAGGACC |
| 851 | ACTTCTGCGC | TCGGCCCTTC | CGGCTGGCTG | GTTTATTGCT | GATAAATCTG |
| 901 | GAGCCGGTGA | GCGTGGGTCT | CGCGGTATCA | TTGCAGCACT | GGGGCCAGAT |
| 951 | GGTAAGCCCT | CCCGTATCGT | AGTTATCTAC | ACGACGGGGA | GTCAGGCAAC |
| 1001 | TATGGATGAA | CGAAATAGAC | AGATCGCTGA | GATAGGTGCC | TCACTGATTA |
| 1051 | AGCATTGGTA | ACTGTCAGAC | CAAGTTTACT | CATATATACT | TTAGATTGAT |
| 1101 | TTAAAACTTC | TTAATTTTAATT | TAAAAGGATC | TAGGTGAAGA | TCCTTTTTGA |
| 1151 | TAATCTCATG | ACCAAAATCC | CTTAACGTGA | | CACTGAGCGT |
| 1201 | CAGACCCCGT | AGAAAAGATC | AAAGGATCTT | | TTTTTTTCTG |
| 1251 | CGCGTAATCT | GCTGCTTGCA | AACAAAAAAA | | CAGCGGTGGT |
| 1301 | TTGTTTGCCG | GATCAAGAGC | TACCAACTCT | TTTTCCGAAG | GTAACTGGCT |
| 1351 | TCAGCAGAGC | GCAGATACCA | AATACTGTCC | TTCTAGTGTA | |
| 1401 | GGCCACCACT | TCAAGAACTC | TGTAGCACCG | CCTACATACC | TCGCTCTGCT |
| 1451 | AATCCTGTTA | CCAGTGGCTG | CTGCCAGTGG | CGATAAGTCG | TGTCTTACCG |
| 1501 | GGTTGGACTC | AAGACGATAG | TTACCGGATA | AGGCGCAGCG | GTCGGGCTGA |
| 1551 | ACGGGGGGTT | CGTGCACACA | GCCCAGCTTG | GAGCGAACGA | |
| 1601 | ACTGAGATAC | : CTACAGCGTG | AGCATTGAGA | . AAGCGCCACG | CTTCCCGAAG |
| 1651 | | : GGACAGGTAT | CCGGTAAGCG | GCAGGGTCGG | |
| 1701 | | AGCTTCCAGG | GGGAAACGCC | TGGTATCTTT | |
| 1751 | | CACCTCTGAC | TTGAGCGTCG | | |
| 1801 | GGGGGCGGAG | CCTATGGAAA | AACGCCAGCA | ACGCGGCCTT | |
| 1851 | | GCTGGCCTTI | TGCTCACATG | TTCTTTCCTG | CGTTATCCCC |
| 1901 | | | TTACCGCCTI | | |
| 1951 | | AACGACCGAG | GCAGCGAGT | CAGTGAGCGA | GGAAGCGGAA |
| | | | | | |

FIG. 13

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| 2001 | GAGCGCCCAA | TACGCAAACC | GCCTCTCCCC | GCGCGTTGGC | CGATTCATTA |
|------|------------|------------|-------------------|------------|------------|
| 2051 | ATGCAGAATT | GATCTCTCAC | CTACCAAACA | ATGCCCCCCT | GCAAAAAATA |
| 2101 | AATTCATATA | AAAAACATAC | AGATAACCAT | CTGCGGTGAT | AAATTATCTC |
| 2151 | TGGCGGTGTT | GACATAAATA | CCACTGGCGG | TGATACTGAG | CACATCAGCA |
| 2201 | GGACGCACTG | ACCACCATGA | AGGTGACGCT | CTTAAAAATT | AAGCCCTGAA |
| 2251 | GAAGGGCAGC | ATTCAAAGCA | GAAGGCTTTG | GGGTGTGTGA | TACGAAACGA |
| 2301 | AGCATTGGCC | GTAAGTGCGA | TTCCGGATTA | GCTGCCAATG | TGCCAATCGC |
| 2351 | GGGGGGTTTT | CGTTCAGGAC | TACAACTGCC | ACACACCACC | AAAGCTAACT |
| 2401 | GACAGGAGAA | TCCAGATGGA | TGCACAAACA | CGCCGCCGCG | AACGTCGCGC |
| 2451 | AGAGAAACAG | GCTCAATGGA | AAGCAGCAAA | TCCCCTGTTG | GTTGGGGTAA |
| 2501 | GCGCAAAACC | AGTTCCGAAA | ${\tt GATTTTTTA}$ | ACTATAAACG | CTGATGGAAG |
| 2551 | CGTTTATGCG | GAAGAGGTAA | AGCCCTTCCC | GAGTAACAAA | AAAACAACAG |
| 2601 | CATAAATAAC | CCCGCTCTTA | CACATTCCAG | CCCTGAAAAA | GGGCATCAAA |
| 2651 | TTAAACCACA | CCTATGGTGT | ATGCATTTAT | TTGCATACAT | TCAATCAATT |
| 2701 | GTTATCCAAG | AAGGAGATAT | ACATATGGGT | CCAGTTCCAC | CATCTACTGC |
| 2751 | TCTGCGTGAA | CTGATTGAAG | AACTGGTTAA | CATCACCCAG | AACCAGAAAG |
| 2801 | CTCCGCTGTG | TAACGGTTCC | ATGGTTTGGT | CCATCAACCT | GACCGCTGGT |
| 2851 | ATGTACTGTG | CAGCTCTGGA | ATCCCTGATC | AACGTTTCTG | GTTGCTCTGC |
| 2901 | TATCGAAAAA | ACCCAGCGTA | TGCTGTCTGG | TTTCTGCCCG | CACAAAGTTT |
| 2951 | CCGCTGGTCA | GTTCTCCTCT | CTGCACGTTC | GTGACACCAA | AATCGAAGTT |
| 3001 | GCTCAGTTCG | TAAAAGACCT | GCTGCTGCAC | CTGAAAAAAC | TGTTCCGTGA |
| 3051 | AGGTCGTTTC | AACTAATAAT | CTAGAGTCGA | CCTGCAGTAA | TCGTACAGGG |
| 3101 | TAGTACAAAT | AAAAAAGGCA | CGTCAGATGA | CGTGCCTTTT | TTCTTGTGAG |
| 3151 | CAGTAAGCTT | GGCACTGGCC | GTCGTTTTAC | AACGTCGTGA | CTGGGAAAAC |
| 3201 | CCTGGCGTTA | CCCAACTTAA | TCGCCTTGCA | GCACATCCCC | CTTTCGCCAG |
| 3251 | CTGGCGTAAT | AGCGAAGAGG | CCCGCACCGA | TCGCCCTTCC | CAACAGTTGC |
| 3301 | GCAGCCTGAA | TGGCGAATGG | CGCCTGATGC | GGTATTTTCT | CCTTACGCAT |
| 3351 | CTGTGCGGTA | TTTCACACCG | CATATATGGT | GCACTCTCAG | TACAATCTGC |
| 3401 | TCTGATGCCG | CATAGTTAAG | CCAGCCCCGA | CACCCGCCAA | |
| 3451 | CGCGCCCTGA | CGGGCTTGTC | TGCTCCCGGC | ATCCGCTTAC | AGACAAGCTG |
| 3501 | TGACCGTCTC | CGGGAGCTGC | ATGTGTCAGA | GGTTTTCACC | GTCATCACCG |
| 3551 | AAACGCGCGA | | | | |

SEQ ID NO:5

FIG. 13 (cont.)

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| 1 | MEWPARLCGL | WALLLCAGGG | GGGGGAAPTE | TQPPVTNLSV | SVENLCTVIW | TWNPPEGASS |
|-----|------------|------------|------------|--------------------|------------|------------|
| 61 | NCSLWYFSHF | GDKQDKKIAP | ETRRSIEVPL | NERICLQVGS | QCSTNESEKP | SILVEKCISP |
| L21 | PEGDPESAVT | ELQCIWHNLS | YMKCSWLPGR | ${\tt NTSPDTNYTL}$ | YYWHRSLEKI | HQCENIFREG |
| 181 | QYFGCSFDLT | KVKDSSFEQH | SVQIMVKDNA | GKIKPSFNIV | PLTSRVKPDP | PHIKNLSFHN |
| 241 | DDLYVQWENP | QNFISRCLFY | EVEVNNSQTE | THNVFYVQEA | KCENPEFERN | VENTSCFMVP |
| | | | | SQEMSIGKKR | | |
| 361 | IVLLLYLKRL | KIIIFPPIPD | PGKIFKEMFG | DQNDDTLHWK | KYDIYEKQTK | EETDSVVLIE |
| 421 | NLKKASQ | | | | | |

SEQ ID NO:12 IL-13Rα1

FIG. 14

